

Supporting Information

Data-guided rational design of additives for halogenation of highly fluorinated naphthalenes: Integrating fluorine chemistry and machine learning

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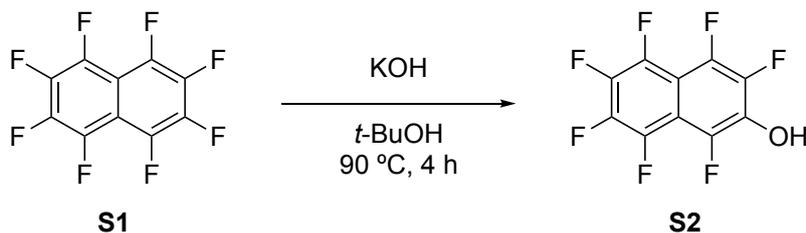
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1. General Information

Unless otherwise noted, all reactions were carried out under an atmosphere of standard grade nitrogen gas (oxygen <10 ppm) in flame-dried glassware with magnetic stirring. Anhydrous THF, CH₂Cl₂, and diethyl ether were supplied from Kanto Chemical Co., Inc. as “Dehydrated solvent system”. Other reagents were purchased from commercial suppliers and used without further purification. Purification of reaction products was carried out by column chromatography on silica gel 60 (spherical, neutral, 100-210 μm; Merck). Analytical thin layer chromatography (TLC) was performed on E. Merck precoated (0.25 mm) silica gel 60-F254 plates. Visualization was accomplished with UV light and a phosphomolybdic acid solution in ethanol by heating. ¹H NMR spectra were recorded on a JEOL ECA-400 (400 MHz) spectrometer at ambient temperature. NMR solvent was purchased from CIL (CDCl₃ and dimethylsulfoxide-d₆). Data are reported as follows: chemical shifts are reported in ppm from tetramethylsilane on the δ scale, with solvent resonance employed as internal standard (CDCl₃ 7.26 ppm, dimethylsulfoxide-d₆ 2.49 ppm), multiplicity (b = broad, s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, and m = multiplet), integration, coupling constant (Hz) and assignment. ¹³C NMR spectra were recorded on a JEOL ECA-400 (100 MHz) or JEOL ECA-600 (151 MHz), spectrometer at ambient temperature. Chemical shifts are reported in ppm from tetramethylsilane on the δ scale, with solvent resonance employed as internal standard (CDCl₃ 77.0 ppm, dimethylsulfoxide-d₆). ¹⁹F NMR spectra were recorded on a JEOL ECS-400 (376 MHz) spectrometer. Chemical shifts are reported in ppm from the α,α,α-trifluorotoluene (–63.72 ppm) resonance as external standard. Infrared (IR) spectra were recorded on a Jasco FT/IR-460 plus using ATR. High-resolution mass spectra (HRMS) analysis was performed on a JEOL JMS-700 (double-focusing magnetic sector mass analyzer: EB) with the fast atom bombardment (FAB) using 3-nitrobenzyl alcohol as the matrix at the Instrument Center, Institute for Molecular Science.

2. Synthesis and characterization of substrates

Synthesis of 1,3,4,5,6,7,8-heptafluoronaphthalen-2-ol (S2)

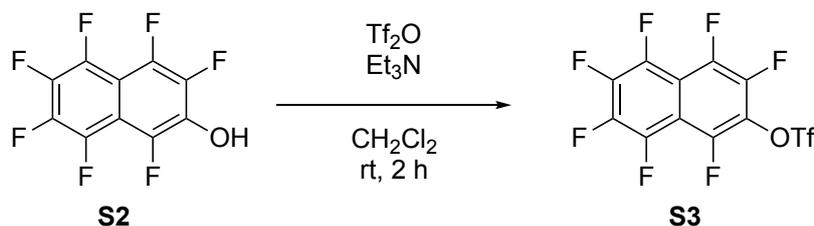


KOH (6.69 g, 119 mmol, 2.0 equiv.) was added to the solution of octafluoronaphthalene **S1** (16.9 g, 59.6 mmol, 1.0 equiv.) in *t*-BuOH (60 mL). The mixture was stirred at 90 °C for 4 h. After cooling to room temperature, H₂O (100 mL) was added to the mixture. The resulting mixture was acidified with 2M HCl aq. (pH <1, 60 mL) and extracted with Et₂O (30 mL×3). The combined organic layer was washed with brine (150 mL), dried over with Na₂SO₄, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane / ethyl acetate = 5:1 as eluent) to give a 1,3,4,5,6,7,8-heptafluoronaphthalen-2-ol **S2** (12.8 g, 47.5 mmol, 79%) as a brown solid.

R_f = 0.18 (hexane / ethyl acetate = 5:1).

¹H NMR (400 MHz, CDCl₃): δ 5.92 (s, 1H). ¹⁹F NMR (376 MHz, CDCl₃): δ -147.1 (ddd, *J* = 57.8, 17.3, 11.5 Hz, 1F), -147.9- -148.3 (m, 2F), -149.3- -149.6 (m, 1F), -153.9 (s, 1F), -156.1 (s, 1F), -158.1 (t, *J* = 18.8 Hz, 1F). ¹³C {¹⁹F} NMR (101 MHz, DMSO-*d*₆): δ 141.2, 140.7, 140.6, 140.4, 139.5, 138.0, 136.7, 135.3, 107.2, 103.0. IR (ATR): 3340, 1660, 1471, 1402, 1196, 1112, 935, 784 cm⁻¹. HRMS(FAB/EB) *m/z* [M]⁺ calcd for C₁₀HF₇O 269.9916, found 269.9922.

Synthesis of 2-[(trifluoromethanesulfonyl)oxy]-1,3,4,5,6,7,8-heptafluoronaphthalene (S3)



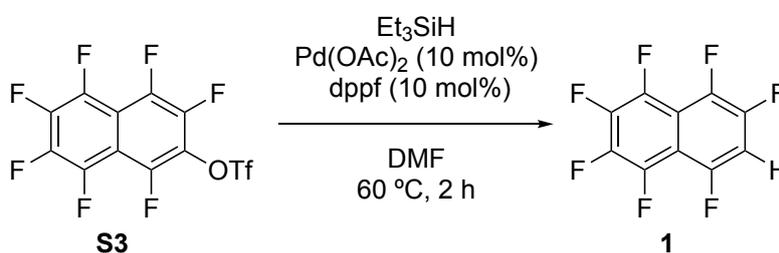
To a solution of 1,3,4,5,6,7,8-heptafluoronaphthalen-2-ol **S2** (6.37 g, 23.6 mmol, 1.0 equiv.) in CH₂Cl₂ (50 mL) was added triethylamine (6.54 mL, 47.2 mmol, 2.0 equiv.) and trifluoromethanesulfonic anhydride (5.80 mL 35.4 mmol, 1.5 equiv.) at 0 °C. The reaction mixture was stirred at room temperature for 2 h. The mixture was quenched with sat. NH₄Cl aq. (50 mL) at 0 °C and extracted with CH₂Cl₂ (30 mL×3). The combined organic layer was washed with brine (150 mL), dried over with Na₂SO₄, and concentrated under reduced pressure after filtration. The crude product was purified by column chromatography on silica gel (hexane / ethyl acetate = 40:1 as eluent)

to give a 2-[(trifluoromethanesulfonyl)oxy]-1,3,4,5,6,7,8-heptafluoronaphthalene **S3** (8.66 g, 21.5 mmol, 91%) as a pale yellow oil.

$R_f = 0.63$ (hexane / ethyl acetate = 5:1).

^{19}F NMR (376 MHz, CDCl_3): δ -73.5 (s, 3F), -132.2 (d, $J = 63.6$ Hz, 1F), -143.5 (dt, $J = 63.6$, 20.2 Hz, 1F), -144.4 (ddd, $J = 56.4$, 20.2, 17.3 Hz, 1F), -144.8 (dt, $J = 60.7$, 17.3 Hz, 1F), -146.9 (s, 1F), -150.6- -150.8 (m, 1F), -151.8 (s, 1F). ^{13}C $\{^{19}\text{F}\}$ NMR (101 MHz, CDCl_3): δ 146.0, 141.7, 141.5, 141.3, 141.0, 140.7, 139.7, 125.4, 118.6, 110.5, 107.3. IR (ATR): 1654, 1458, 1412, 1216, 1122, 948, 823, 778, 726, 697 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}]^+$ calcd for $\text{C}_{11}\text{F}_{10}\text{SO}_3$ 401.9408, found: 401.9408.

Synthesis of F_7 naphthalene (**1**)

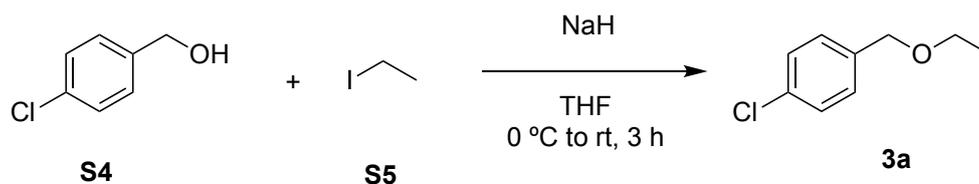


To a solution of 2-[(trifluoromethanesulfonyl)oxy]-1,3,4,5,6,7,8-heptafluoronaphthalene **S3** (10.0 g, 24.9 mmol, 1.0 equiv.) in DMF (50 mL) was added Et_3SiH (20.0 mL, 124 mmol, 5.0 equiv.), dppf (1.38 g, 2.49 mmol, 10 mol%) and $\text{Pd}(\text{OAc})_2$ (555 mg, 2.49 mmol, 10 mol %) at $0\text{ }^\circ\text{C}$. After stirring at $0\text{ }^\circ\text{C}$ for 10 min, the reaction mixture was allowed warm to $60\text{ }^\circ\text{C}$ and stirred for 2 h. After cooling to room temperature, H_2O (60 mL) was added to the mixture, then the resulting suspension was filtered through a pad of Celite while washing with Et_2O (30 mL). The filtrate was extracted with Et_2O (30 mL \times 3). The combined organic layer was washed with H_2O (100 mL) and brine (150 mL), dried over Na_2SO_4 , and concentrated under reduced pressure after the filtration. The crude product was purified by column chromatography on silica gel (hexane 100% as eluent) to give F_7 naphthalene (**1**) (5.37 g, 21.2 mmol, 85%) as a white solid.

$R_f = 0.45$ (hexane).

^1H NMR (400 MHz, CDCl_3): δ 7.18 (dt, $J = 10.4$, 5.8 Hz, 1H). ^{19}F NMR (376 MHz, CDCl_3): δ -117.1- -117.4 (m, 1F), -134.5- -134.7 (m, 1F), -145.0 (dt, $J = 63.6$, 17.3 Hz, 1F), -146.7 (dt, $J = 58.8$, 16.6 Hz, 1F), -150.2- -150.5 (m, 1F), -153.8 (dd, $J = 21.7$, 15.9 Hz, 1F), -155.6 (dd, $J = 21.7$, 15.9 Hz, 1F). ^{13}C $\{^{19}\text{F}\}$ NMR (101 MHz, CDCl_3): δ 152.6 (d, $J = 6.7$ Hz), 146.8 (d, $J = 6.7$ Hz), 141.4, 141.3, 140.4 (d, $J = 6.7$ Hz), 139.9, 138.5, 112.2, 108.2 (d, $J = 5.8$ Hz), 104.9 (d, $J = 168.7$ Hz). IR (ATR): 1650, 1401, 1138, 923, 845, 781, 701 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}]^+$ calcd for C_{10}HF_7 263.9966, found 263.9967.

Synthesis of 1-chloro-4-(1-ethoxymethyl)benzene (**3a**)^{S1}



NaH (260 mg, 6.50 mmol, 1.3 equiv.) was charged with 50 mL two neck round bottom flask. The flask was purged with a nitrogen gas. THF (10 mL) was added to the flask and cooled to 0 °C. 4-chlorobenzyl alcohol **S4** (713 mg, 5.00 mmol, 1.0 equiv.) was added to the resulting suspension. The mixture was stirred at 0 °C for 30 min. Iodoethane **S5** (520 μ L, 6.50 mmol, 1.3 equiv.) was added dropwise to the mixture. The resulting mixture was allowed warm to room temperature and stirred for 3 h. The mixture was quenched with H₂O (15 mL) and extracted with diethyl ether (10 mL \times 3). The combined organic layer was dried over Na₂SO₄ and concentrated under reduced pressure after filtration. The residual crude product was purified by column chromatography on silica gel (hexane/ethyl acetate = 20:1) to afford a 1-chloro-4-(1-ethoxymethyl)benzene **3a** as a colorless oil (242 mg, 1.40 mmol, 28%).

R_f = 0.55 (hexane/ethyl acetate = 10:1).

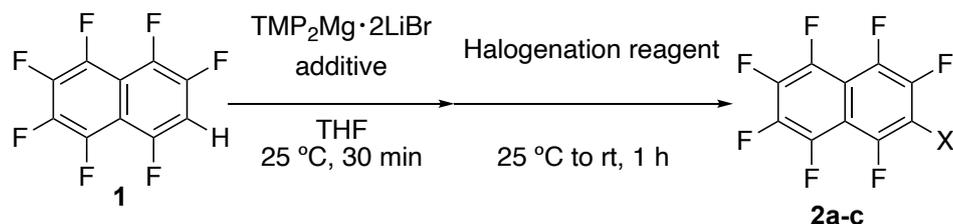
¹H NMR (400 MHz, CDCl₃): δ 7.33-7.26 (m, 4H), 4.47 (s, 2H), 3.53 (q, J = 7.1 Hz, 2H), 1.24 (t, J = 7.1 Hz, 3H).

3. Preparation of $\text{TMP}_2\text{Mg}\cdot 2\text{LiBr}^{\text{S2}}$

A 30 mL two-neck round-bottomed flask was charged with Mg powder (122 mg, 5.00 mmol, 1.0 equiv.). The flask was flame-dried under vacuo. Then, the flask was backfilled with nitrogen gas three times. THF (5.0 mL) and 1,2-dibromoethane (430 μL , 5.00 mmol, 1.0 equiv.) were added to the flask at room temperature. The mixture was refluxed for 1 h to give a MgBr_2 in THF. In another 30 mL two neck flask, 2,2,6,6-tetramethylpiperidine (1.70 mL, 10.0 mmol, 2.0 equiv.) and THF (5.0 mL) were charged. After cooling to $-78\text{ }^\circ\text{C}$, *n*-BuLi (1.58 M in hexane, 6.33 mL, 10.0 mol, 2.0 equiv.) was added dropwise to the solution at $-78\text{ }^\circ\text{C}$. The resulting mixture was warmed to $0\text{ }^\circ\text{C}$ and stirred for 30 min. The resulting solution was transferred to the MgBr_2 in THF via cannula at $0\text{ }^\circ\text{C}$. The mixture was stirred at $0\text{ }^\circ\text{C}$ for 30 min, then warmed to room temperature and stirred for 30 min to afford a $\text{TMP}_2\text{Mg}\cdot 2\text{LiBr}$ (0.24 M in THF) as a light brown solution. The $\text{TMP}_2\text{Mg}\cdot 2\text{LiBr}$ was titrated at $0\text{ }^\circ\text{C}$ against benzoic acid using 4-phenylazodiphenylamine as indicator.

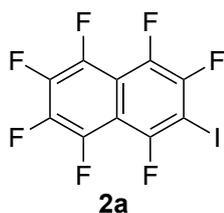
4. Halogenation of F_7 naphthalene (**1**) in the presence of additive

General procedure:



F_7 naphthalene (**1**) (51.0 mg, 0.200 mmol, 1.0 equiv.) and corresponding additive (1.0 equiv.) were dissolved in THF (1.5 mL). $\text{TMP}_2\text{Mg}\cdot 2\text{LiBr}$ (0.24 M in THF, 1.00 mL, 0.240 mmol, 1.2 equiv.) was added to the solution at $25\text{ }^\circ\text{C}$. The mixture was stirred at $25\text{ }^\circ\text{C}$ for 30 min, then corresponding halogenation reagent was added to the reaction mixture. The mixture was stirred at $25\text{ }^\circ\text{C}$ for 1 h, quenched with 2 M HCl aq. (5 mL) at $0\text{ }^\circ\text{C}$ and extracted with Et_2O (10 mL \times 3). The combined organic layer was washed with sat. Na_2SO_3 aq. (5 mL) and brine (5 mL), dried over Na_2SO_4 , and concentrated under reduced pressure after filtration. The residual crude product was dissolved in CDCl_3 . Dibromomethane (14 μL , 0.200 mmol, 1.0 equiv.) and hexafluorobenzene (23 μL , 0.200 mmol, 1.0 equiv.) were added to the solution, then ^1H and ^{19}F NMR was taken to determine the yield of **2** and recovery of additive.

Characterization of 1,2,3,4,5,6,8-Heptafluoro-7-iodonaphthalene (**2a**)

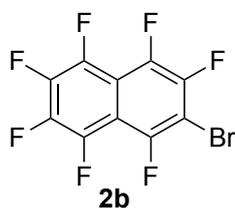


The **2a** was synthesized according to general procedure using molecular iodine (122 mg, 0.480 mmol, 2.4 equiv.) as halogenation reagent and **3a** (31 μ L, 0.200 mmol, 1.0 equiv.) as additive. **2a** was obtained in 96% NMR yield and **3a** was recovered in 96% yield.

R_f = 0.43 (hexane).

^{19}F NMR (376 MHz, CDCl_3): δ -96.9 (dd, J = 66.5, 17.3 Hz, 1F), -116.4- -116.5 (m, 1F), -144.1 (dt, J = 66.5, 17.3 Hz, 1F), -146.3 (dt, J = 59.7, 16.6 Hz, 1F), -147.0- -147.3 (m, 1F), -152.9- -153.1 (m, 1F), -155.1 (s, 1F). ^{13}C $\{^{19}\text{F}\}$ NMR (101 MHz, CDCl_3): δ 152.9, 147.0, 141.4, 140.6, 140.1, 139.8, 138.8, 111.7, 107.7, 72.7. IR (ATR): 1650, 1487, 1399, 1254, 1161, 1107, 946, 889, 739, 686, 665 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}]^+$ calcd for $\text{C}_{10}\text{F}_7\text{I}$ 379.8933, found 379.8932.

2-Bromo-1,3,4,5,6,7,8-heptafluoronaphthalene (**2b**)

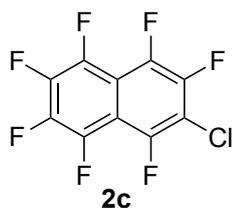


2b was synthesized according to general procedure using Br_2 (51 μ L, 1.00 mmol, 5.0 equiv.) as halogenation reagent and **3a** (31 μ L, 0.200 mmol, 1.0 equiv.) as additive. **2b** was obtained in 95% NMR yield, and **3a** was recovered in 94% yield.

R_f = 0.44 (hexane).

^{19}F NMR (376 MHz, CDCl_3): δ -111.4 (dd, J = 66.5, 14.4 Hz, 1F), -128.6- -128.8 (m, 1F), -144.4 (dt, J = 66.5, 17.3 Hz, 1F), -146.1 (dt, J = 59.7, 15.9 Hz, 1F), -146.7- -147.1 (m, 1F), -153.1 (dd, J = 20.2, 17.3 Hz, 1F), -154.7 (dd, J = 23.1, 14.5 Hz, 1F). ^{13}C $\{^{19}\text{F}\}$ NMR (101 MHz, CDCl_3): δ 150.2, 145.1, 141.4, 140.7, 140.7, 139.9, 139.0, 110.7, 107.9, 99.6. IR (ATR): 1638, 1522, 1483, 1398, 1252, 1156, 1106, 948, 897, 744 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}]^+$ calcd for $\text{C}_{10}\text{BrF}_7$ 331.9072, found 331.9062.

2-Chloro-1,3,4,5,6,7,8-heptafluoronaphthalene (**2c**)



2c was synthesized according to general procedure using PhSO_2Cl (76 μL , 0.600 mmol, 3.0 equiv.) as halogenation reagent and **3a** (31 μL , 0.200 mmol, 1.0 equiv.) as additive. **2c** was obtained in 96% NMR yield and **3a** was recovered in 96% yield.

$R_f = 0.50$ (hexane).

^{19}F NMR (376 MHz, CDCl_3): δ -120.1 (dd, $J = 66.5, 17.3$ Hz, 1F), -136.1- -136.2 (m, 1F), -144.6 (dt, $J = 64.5, 16.6$ Hz, 1F), -146.0 (dt, $J = 59.7, 16.6$ Hz, 1F), -146.9- -147.1 (m, 1F), -153.1- -153.3 (m, 1F), -154.6- -154.7 (m, 1F). ^{13}C $\{^{19}\text{F}\}$ NMR (101 MHz, CDCl_3): δ 149.3, 144.4, 141.3, 141.0, 140.9, 139.8, 139.1, 111.4, 109.9, 107.7. IR (ATR): 1639, 1477, 1393, 1162, 1105, 916, 750 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}]^+$ calcd for $\text{C}_{10}\text{ClF}_7$ 287.9577, found 287.9585.

List of additives from FG-kit^{S3}

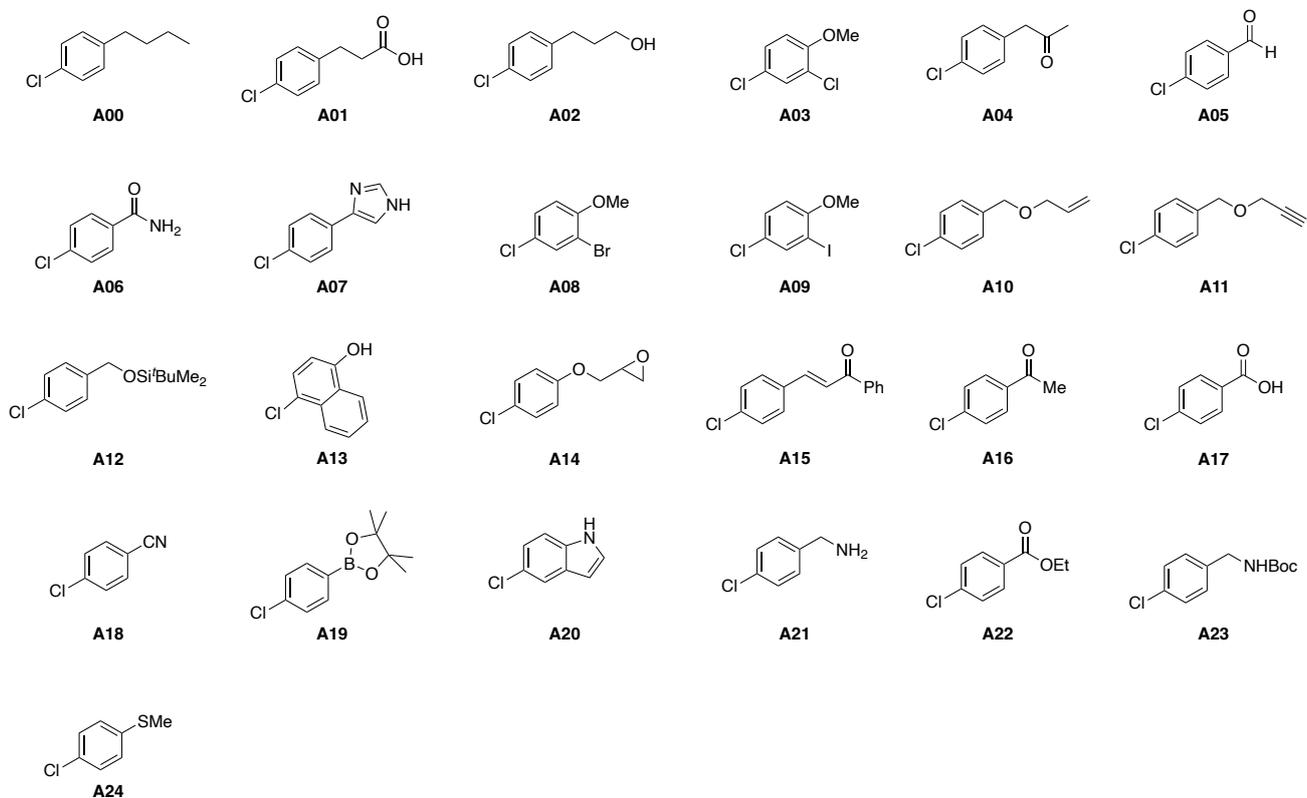
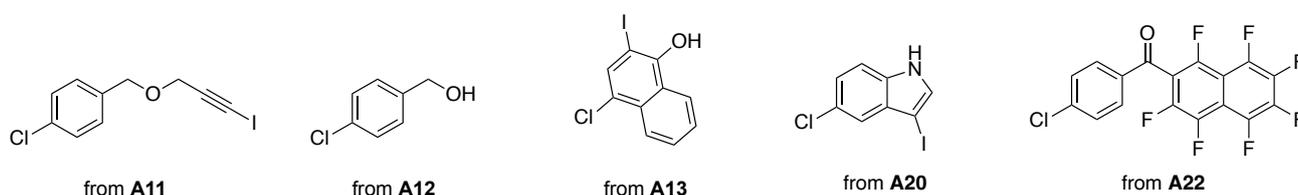


Figure S1. List of chemical structure of all additives from FG-kit

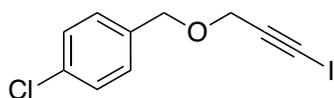
Table S1. Results of additive effect in iodination of heptafluoronaphthalene

 A00 2 82% yield Additive 99% yield	 A01 2 0% yield Additive 65% yield	 A02 2 0% yield Additive 88% yield	 A03 2 0% yield Additive 74% yield	 A04 2 0% yield Additive 0% yield
 A05 2 0% yield Additive 22% yield	 A06 2 0% yield Additive 70% yield	 A07 2 0% yield Additive 0% yield	 A08 2 0% yield Additive 81% yield	 A09 2 20% yield Additive 95% yield
 A10 2 94% yield Additive 70% yield	 A11 2 96% yield Additive 0% yield	 A12 2 0% yield Additive 56% yield	 A13 2 0% yield Additive 0% yield	 A14 2 0% yield Additive 0% yield
 A15 2 0% yield Additive 0% yield	 A16 2 0% yield Additive 0% yield	 A17 2 0% yield Additive 65% yield	 A18 2 7% yield Additive 32% yield	 A19 2 34% yield Additive 50% yield
 A20 2 0% yield Additive 0% yield	 A21 2 87% yield Additive 19% yield	 A22 2 0% yield Additive 0% yield	 A23 2 8% yield Additive 68% yield	 A24 2 73% yield Additive 87% yield

The reaction was carried out using 0.200 mmol of **1**, 0.240 mmol of $\text{TMP}_2\text{Mg}\cdot 2\text{LiBr}$, and 0.200 mmol of additive in THF (1.5 mmol). The yield of **2** and recovery of additive are determined by ^1H and ^{19}F NMR using dibromomethane and hexafluorobenzene as an internal standard. In several cases, by-product derived from reactions of the additives were observed, as shown below.



· Characterization of by-products

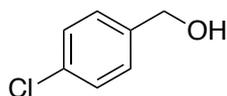


from **A11**

Light brownish oil.

$R_f = 0.53$ (hexane/ethyl acetate = 5:1)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.36-7.26 (m, 4H), 4.56 (s, 2H), 4.32 (s, 1H). ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 135.7, 133.7, 129.4, 128.6, 128.2, 90.1, 70.9, 58.8. IR (ATR): 2926, 2852, 1492, 1348, 1086, 1014, 906, 799, 729 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}-\text{H}]^+$ calcd for $\text{C}_{10}\text{H}_7\text{ClOI}$ 304.9230, found 304.9244.



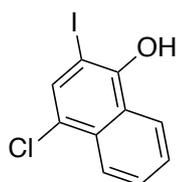
from **A12**

White solid

$R_f = 0.30$ (hexane/ethyl acetate = 3:1)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.29-7.22 (m, 4H), 4.58 (s, 2H), 2.43 (brs, 1H).

This is known compound and the spectroscopic data is agreement with the literature.^{S2}

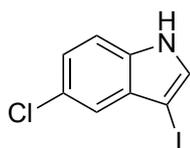


from **A13**

Brownish semi solid

$R_f = 0.33$ (hexane/ethyl acetate = 3:1)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.27 (d, $J = 8.5$ Hz, 1H), 8.17 (d, $J = 8.5$ Hz, 1H), 7.73 (s, 1H), 7.66-7.62 (m, 1H), 7.62-7.54 (m, 1H), 5.71 (s, 1H). ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 150.6, 132.5, 131.3, 128.0, 126.8, 125.9, 124.5, 123.0, 122.4, 102.8. IR (ATR): 3270, 2975, 1575, 1374, 1054, 1034, 1024, 819, 757, 684 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{10}\text{H}_7\text{ClOI}$ 304.9230, found 304.9224



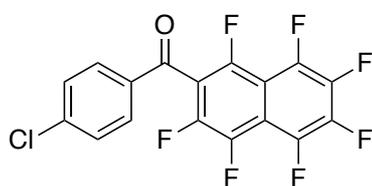
from **A20**

White solid

$R_f = 0.30$ (hexane/ethyl acetate = 4:1)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.29 (s, 1H), 7.43 (d, $J = 1.0$ Hz, 1H), 7.30–7.19 (m, 2H), 7.16 (dd, $J = 8.6, 1.8$ Hz, 1H).

This is known compound and the spectroscopic data is agreement with the literature.^{S3}



from **A22**

Light yellow oil

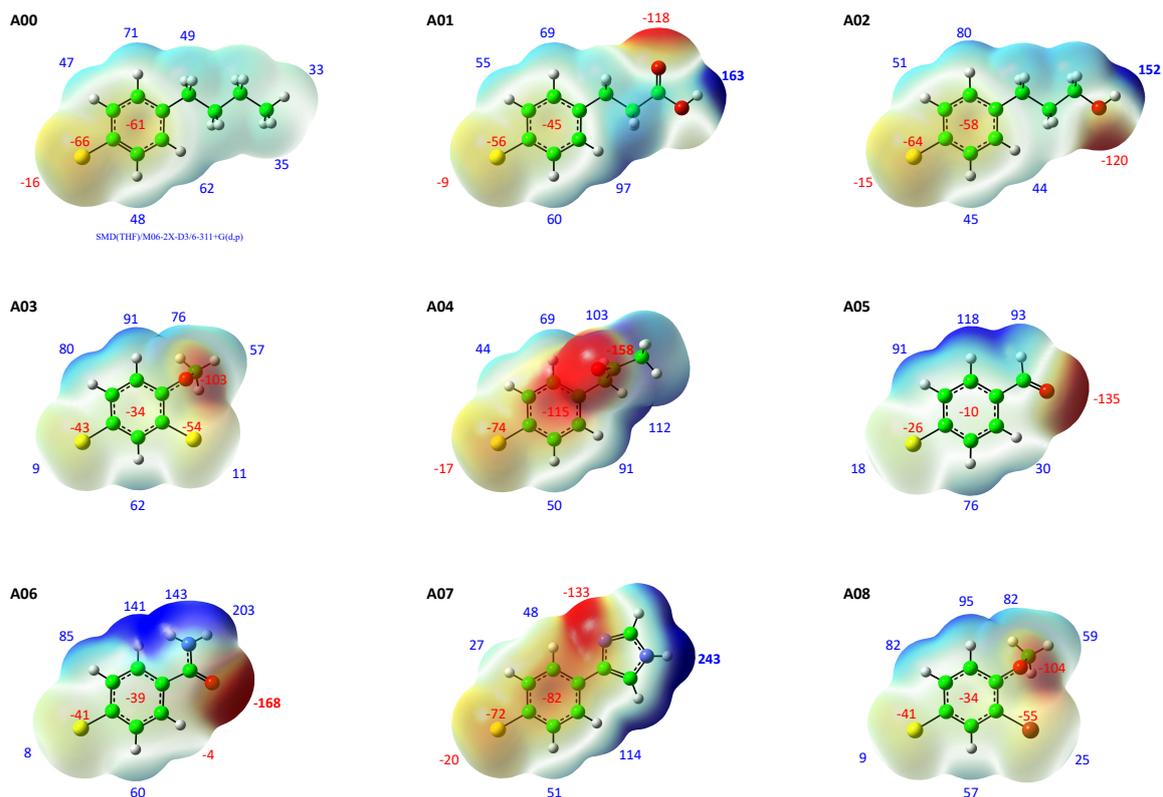
$R_f = 0.40$ (hexane/ethyl acetate = 5:1)

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.42–7.37 (m, 4H), $^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ –115.3 (dd, $J = 78.0, 17.3$ Hz, 1F), –133.8 (s, 1F), –142.3 (dt, $J = 78.0, 17.3$ Hz, 1F), –145.4 (dt, $J = 57.8, 14.5$ Hz, 1F), –147.0 (dt, $J = 57.8, 17.3$ Hz, 1F), –151.2 (t, $J = 17.3$ Hz, 1F), –153.9 (t, $J = 20.2$ Hz, 1F) ^{13}C { ^{19}F } NMR (101 MHz, CDCl_3): δ 150.4, 149.6, 146.0, 144.9, 141.9, 141.3, 140.9, 140.8–140.4 (m), 140.3, 139.1, 135.2 (d, $J = 8.6$ Hz), 129.1 (d, $J = 170.6$ Hz), 127.4 (d, $J = 156.2$ Hz), 121.3, 111.4, 108.0. IR (ATR): 1653, 1490, 1404, 1161, 1113, 945, 931, 730, 597 cm^{-1} . HRMS (FAB/EB) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_5\text{ClOF}_7$ 392.9917, found 392.9921.

5. DFT calculation

All molecular geometries were optimized by the M06-2X functional with Grimme's D3 dispersion correction^{S6} using the SDD basis set (iodine) and 6-311+G(d,p) for all other atoms. The SMD18 solvation model^{S7,S8} was used with THF as the solvent. The stationary geometries were checked by the vibration analyses after the geometry optimization procedures. The stationary geometries and their energies were refined using Gaussian 16 software package.^{S9}

5-1. Electrostatic Potential Map of additives



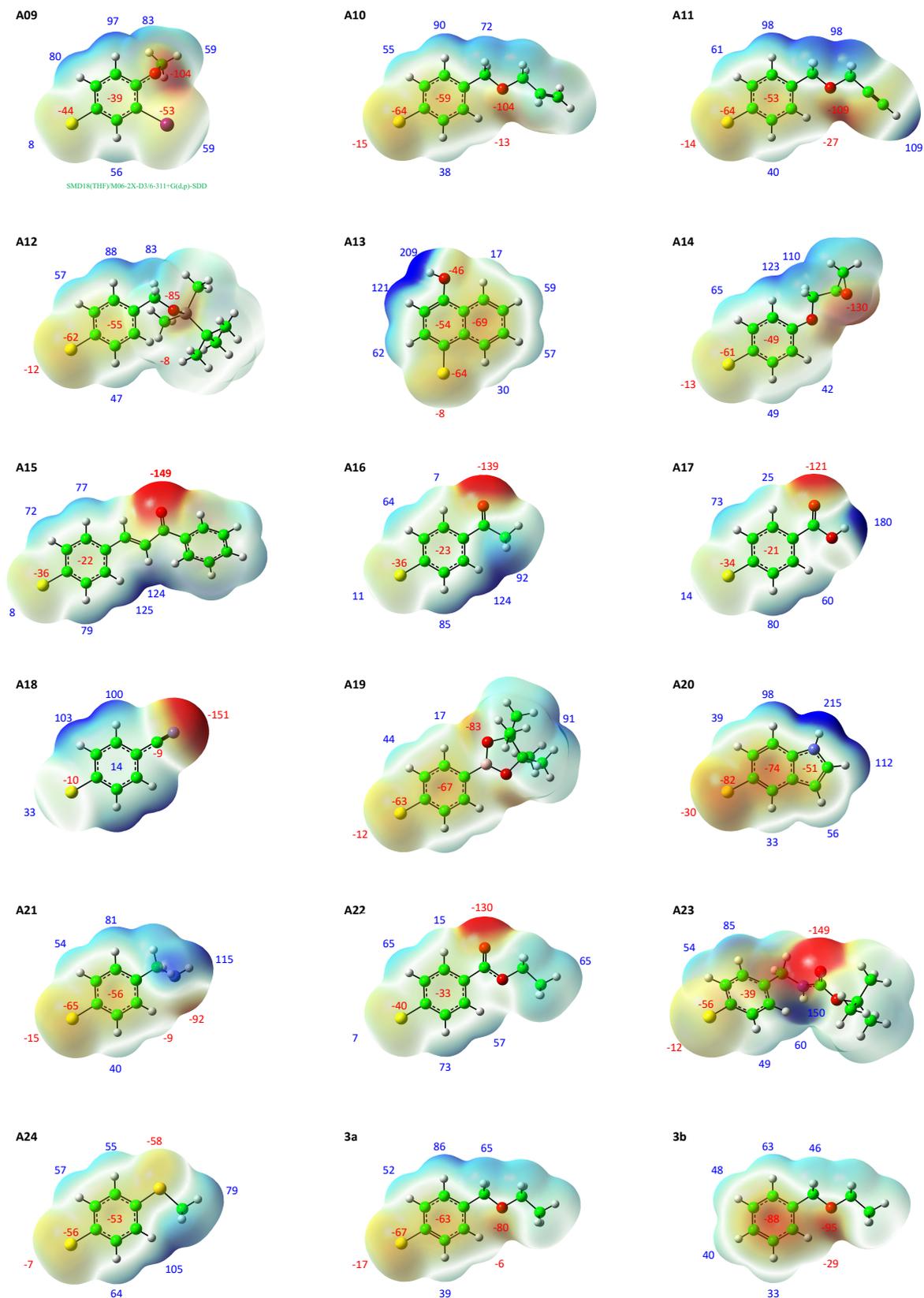
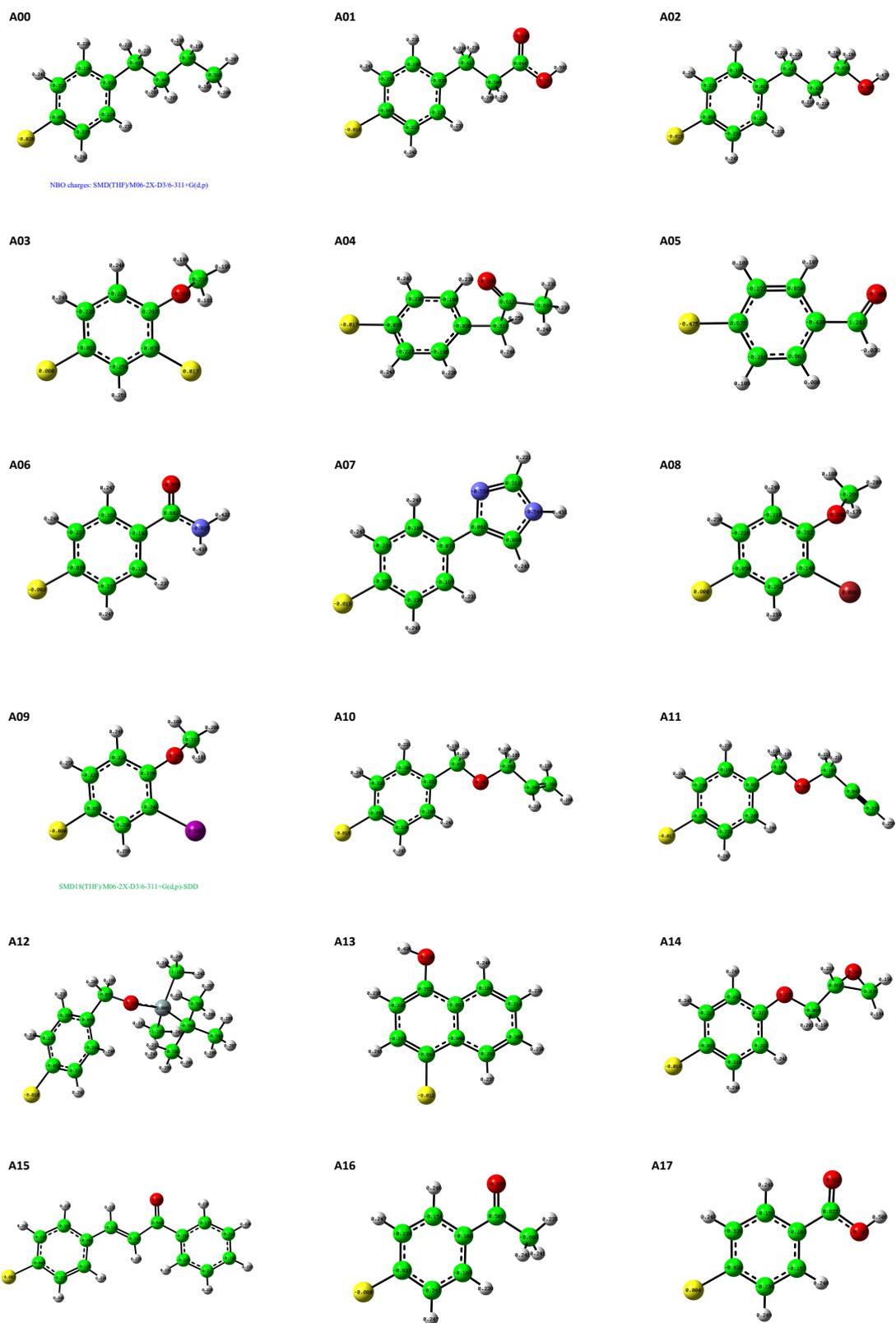


Figure S2. Molecular electrostatic potential maps and each energy value ($\text{kJ}\cdot\text{mol}^{-1}$) of **additives (A0-A24, 3a, and 3b)**. Optimized geometries were calculated at the SMD18(THF)/M06-2X-D3/6-311+G(d,p) or SMD18(THF)/M06-2X-D3/6-311+G(d,p)-SDD level.

5-2. NBO charge of additives



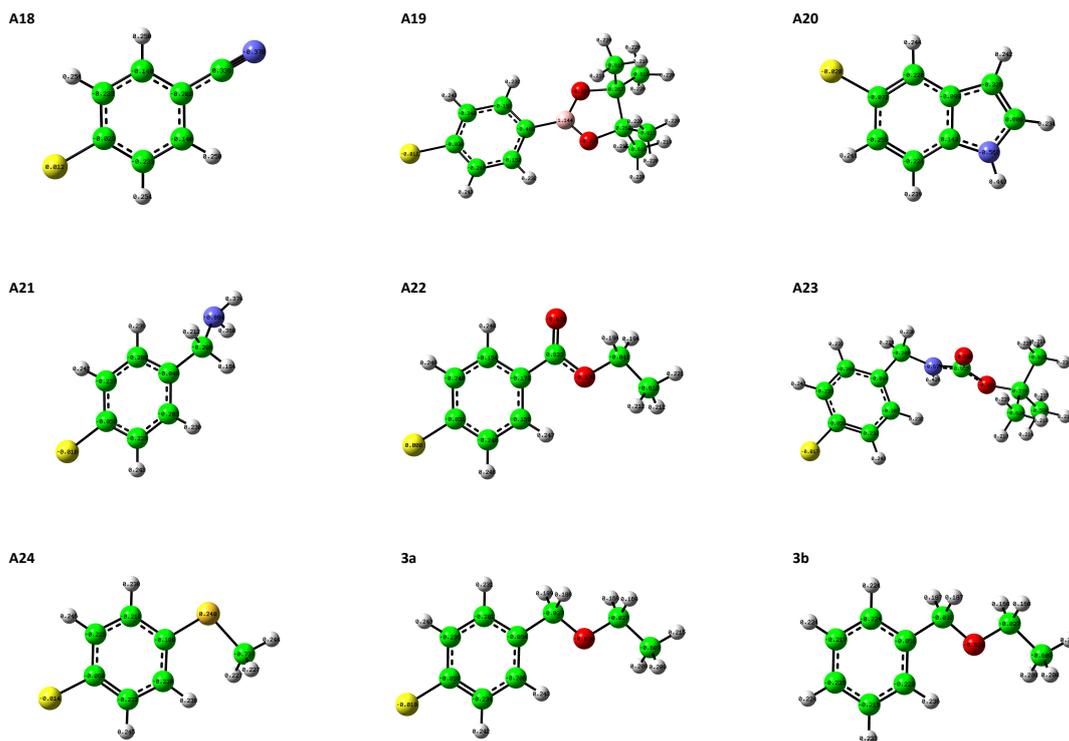


Figure S3. NBO charge of additives (A0-A24, 3a, and 3b). Optimized geometries were calculated at the SMD18(THF)/M06-2X-D3/6-311+G(d,p) or SMD18(THF)/M06-2X-D3/6-311+G(d,p)-SDD level.

5-3. Geometry optimization of 3a···F₇MgTMP complex

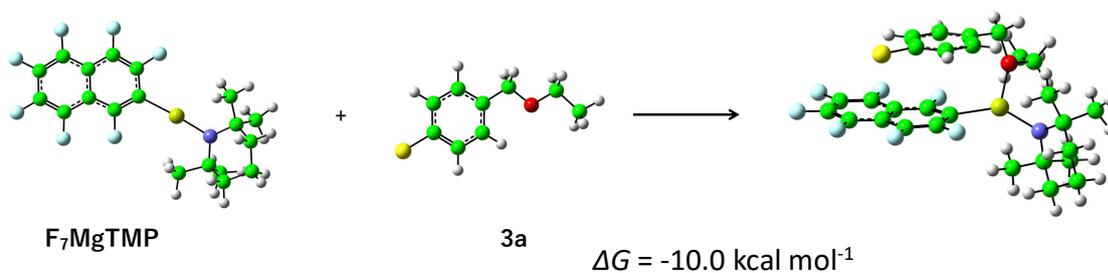


Figure S4. Geometry optimization and Gibbs free energy in formation of F₇MgTMP···3a complex. Optimized geometries were calculated at the SMD18(THF)/M06-2X-D3/6-311+G(d,p)

Computational Details.

The table S2 shows total energy E , enthalpy H , and Gibbs free energy G (hartree) at the SMD18(THF)/M06-2X-D3/6-311+G(d,p)-SDD level.

Table S2 Total energy E , enthalpy H , and Gibbs free energy G (hartree) of **3a**, F₇MgTMP and **3a**···F₇MgTMP complex at the SMD18(THF)/M06-2X-D3/6-311+G(d,p)-SDD level.

	E	H	G
3a	-884.932251	-884.739330	-884.791045
F ₇ MgTMP	-1688.466609	-1688.098923	-1688.184233
3a ···F ₇ MgTMP	-2573.441341	-2572.878200	-2572.991221

5-4. IGMH analysis, ESP map, and NBO charge of **3a**···F₇MgTMP complex

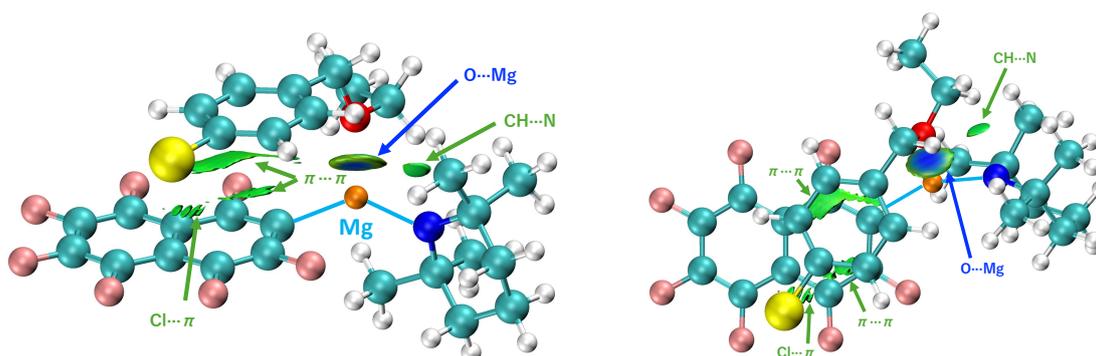


Figure S5. IGMH map of the calculated complex. (left) side view. (right) top view.

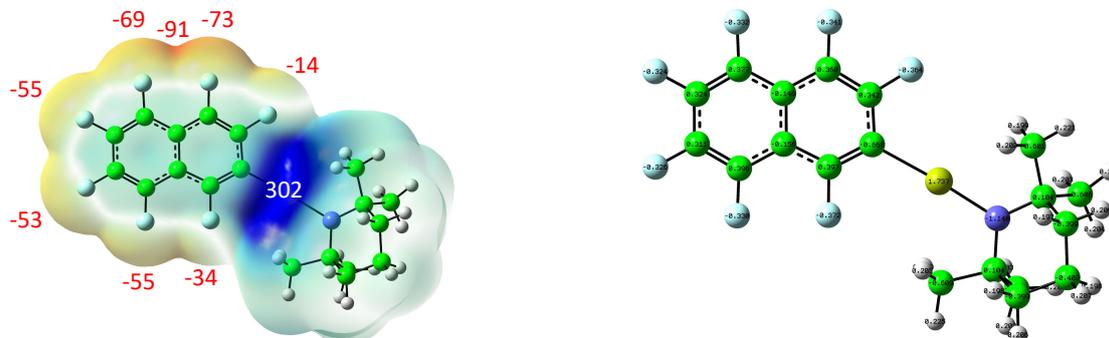


Figure S6. Molecular electrostatic potential maps and each energy value (kJ·mol⁻¹), and NBO charge of the calculated complex.

6. Machine learning

6-1. Preparation of data set

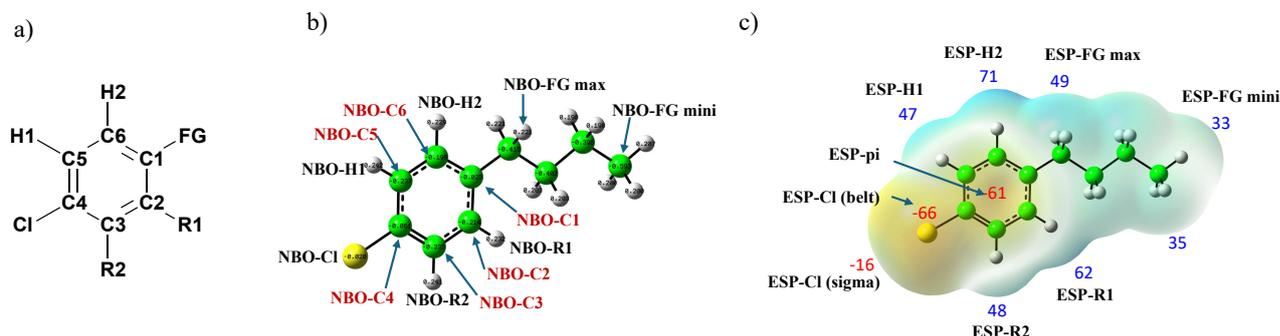


Figure S7. Definition of electronic descriptors used in the machine learning analysis (example additive; **A00**). (a) Common structure of the additive and the atom numbering used in descriptor calculation. (b) Representative NBO charges for **A00** used as input features (c) Electrostatic potential (ESP) map for **A00** highlighting key ESP descriptors employed in the model

Table S3. List of descriptors

Descriptor	Mean of descriptor
Yield	Yield of compound 2
NBO-Cl	NBO charge on the chlorine atom
NBO-R1	NBO charge on R1
NBO-R2	NBO charge on R2
NBO-H1	NBO charge on H1
NBO-H2	NBO charge on H2
NBO-C1	NBO charge on C1
NBO-C2	NBO charge on C2
NBO-C3	NBO charge on C3
NBO-C4	NBO charge on C4
NBO-C5	NBO charge on C5
NBO-C6	NBO charge on C6
NBO-FG mini	Minimum NBO charge within the functional group
NBO-FG max	Maximum NBO charge within the functional group
ESP-Cl (sigma)	Electrostatic potential at the σ -hole of the chlorine atom
ESP-Cl (belt)	Electrostatic potential at the negative belt of the chlorine atom
ESP-pi	Electrostatic potential at the center of aromatic ring
ESP-R1	Electrostatic potential at R1

ESP-R2	Electrostatic potential at of R2
ESP-H1	Electrostatic potential at of H1
ESP-H2	Electrostatic potential at of H2
ESP-FG mini	Minimum electrostatic potential within functional group
ESP-FG max	Maximum electrostatic potential within functional group

6-2. Correlation analysis

Correlation analysis was performed by Datachemical Lab^{S10} using the prepared datasets. The Pearson correlation coefficient is calculated using the following equation.^{S11}

$$r = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}}$$

n = Number of data point, x_i and y_i = Individual values, \bar{x} and \bar{y} = Mean values

The correlation strength was classified according to the following absolute value ranges of the correlation coefficient: very high, $0.9 < |r| < 1$; high, $0.7 < |r| < 0.9$; moderate, $0.5 < |r| < 0.7$; low, $0.3 < |r| < 0.5$; weak, $|r| < 0.3$.^{S9}

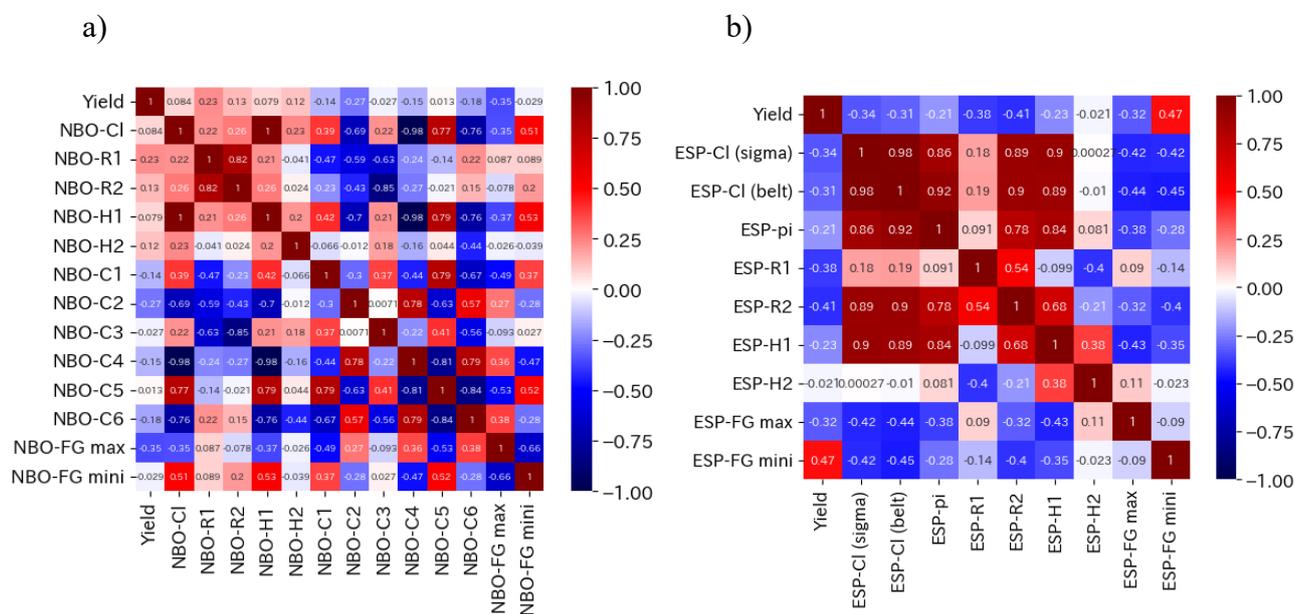


Figure S8. Heatmap and Pearson correlation coefficient. a) correlation between yield and NBO charge. b) correlation between yield and Electrostatic potential.

6-3. Regression analysis

Model evaluation was carried out using Datachemical Lab. The dataset was randomly divided into training (75%) and test (25%) sets with 5-fold cross-validation.

Table S4. Accuracy of all prediction model.

model		r2(test)	RMSE(test)	MAE(test)
NSVR	Nonlinear Support Vector Regression	0.89847579	10.900329	10.3915414
NGPR3	Nonlinear Gaussian Process Regression 3	0.85068412	13.2192795	11.1011724
NGPR5	Nonlinear Gaussian Process Regression 5	0.77169322	16.3461014	14.6168611
DT	Decision Tree	0.76642358	16.5336708	11.1527778
NGPR9	Nonlinear Gaussian Process Regression 9	0.74919768	17.132493	15.0836416
NGPR7	Nonlinear Gaussian Process Regression 7	0.73669037	17.5544878	15.4789745
NGPR1	Nonlinear Gaussian Process Regression 1	0.7193678	18.1227267	15.6533991
NGPR2	Nonlinear Gaussian Process Regression 2	0.71871111	18.143918	15.6741789
RF	Random Forests	0.61452212	21.2400002	16.9893333
NGPR4	Nonlinear Gaussian Process Regression 4	0.478212	24.711655	16.9490438
GBDT	Gradient Boosting Decision Tree	0.35123675	27.5548409	19.501895
XGB	eXtream Gradient Boosting	0.30349952	28.5506169	19.6167576
VBGMR	Variational Bayesian Gaussian Mixture Regression	-0.0304017	34.7262654	25
GMR	Gaussian Mixture Regression	-0.0883178	35.6888588	25
DNN	Deep Neural Network	-1.4128288	53.1395704	41.6259043
LASSO	Least Absolute Shrinkage and Selection Operator	-1.444762	53.4900593	44.6101112
EN	Elastic Net	-3.0547998	68.8873525	56.7776412
RR	Ridge Regression	-3.597467	73.3523612	59.8705876
LGPR	Linear Gaussian Process Regression	-4.4412687	79.8003641	63.0195761
NGPR10	Nonlinear Gaussian Process Regression 10	-4.4412826	79.8004664	63.0196222
NGPR8	Nonlinear Gaussian Process Regression 8	-4.4412921	79.800536	63.0196536
NGPR6	Nonlinear Gaussian Process Regression 6	-4.4412933	79.8005444	63.0196574
LSVR	Linear Support Vector Regression	-5.0649415	84.2496479	64.5706272
PLS	Partial Least Squares regression	-5.3931069	86.498937	67.5108526
OLS	Ordinary Least Squares regression	-51359.174	7752.96869	4531.05375

* NGPR 1–10 employ different kernel functions.

Cross-validated Permutation Feature Importance (CVPMFI) in Non-linear support vector regression (NSVR) is shown in Table S5.

Table S5. List of CVPFI in NSVR model.

Name	mean	std
NBO-FG max	0.23617102	0.06500494
ESP-FG mini	0.19710634	0.12976835
ESP-FG max	0.15751688	0.1976209
ESP-R1	0.12129823	0.1448446
ESP-R2	0.10707701	0.04177292
ESP-C1 (sigma)	0.1022561	0.05829173
ESP-C1 (belt)	0.07834765	0.04165044
NBO-R1	0.05486647	0.03464369
NBO-H2	0.03900008	0.08646733
NBO-H1	0.0387144	0.07773518
NBO-C6	0.03562281	0.05693992
NBO-C4	0.03456521	0.04920815
NBO-C1	0.02708324	0.0555702
NBO-C1	0.02452407	0.03594442
ESP-H1	0.02204522	0.05035651
ESP-pi	0.01293239	0.03777208
NBO-R2	0.0103235	0.07685471
ESP-H2	-0.002851	0.01817305
NBO-C3	-0.0036538	0.03833801
NBO-C2	-0.0043658	0.02454139
NBO-C5	-0.012673	0.03690806
NBO-FG mini	-0.0925581	0.02824967

Table S6 summarizes the predicted yields of additives **3a** and **3b** obtained from the optimized NSVR model, together with the standardized response values and applicability domain (AD) scores. AD score was evaluated using the k-nearest neighbors (k-NN) approach as implemented in Datachemical Lab.

Table S6

Additive	estimated yield	sum of standardized y	AD
3a	101.3888666	0.039747553	0.256666304
3b	41.18933845	1.683084574	0.067922676

6-4. SHAP Analysis for Feature Contribution

To interpret the contribution of each molecular descriptor to the predicted reaction yield, SHAP (SHapley Additive exPlanations) analysis was performed based on a nonlinear support vector regression (NSVR) model. The NSVR model employed a radial basis function (RBF) kernel to capture nonlinear relationships between molecular descriptors and the reaction yield.

Hyperparameters (C, epsilon, gamma) were optimized via a grid search with 5-fold cross-validation. Prior to model training, all descriptor values were standardized using StandardScaler from scikit-learn. The dataset was randomly divided into training and test sets (75%/25%), and hyperparameter tuning for the NSVR model was carried out using a grid search with 5-fold cross-validation. ($R^2 = 0.86$, MAE = 11.96, RMSE = 14.68)

Using the optimized model, SHAP values were computed for the prediction of reaction yield using the shap Python package, enabling visualization of global and individual feature importance.

The following Python packages were used:

Python (v3.11.5), pandas (v2.2.3), numpy (v2.1.3), scikit-learn (v1.6.1), shap (v0.46.1)

6-4-1. SHAP analysis for additives using NSVR as model.

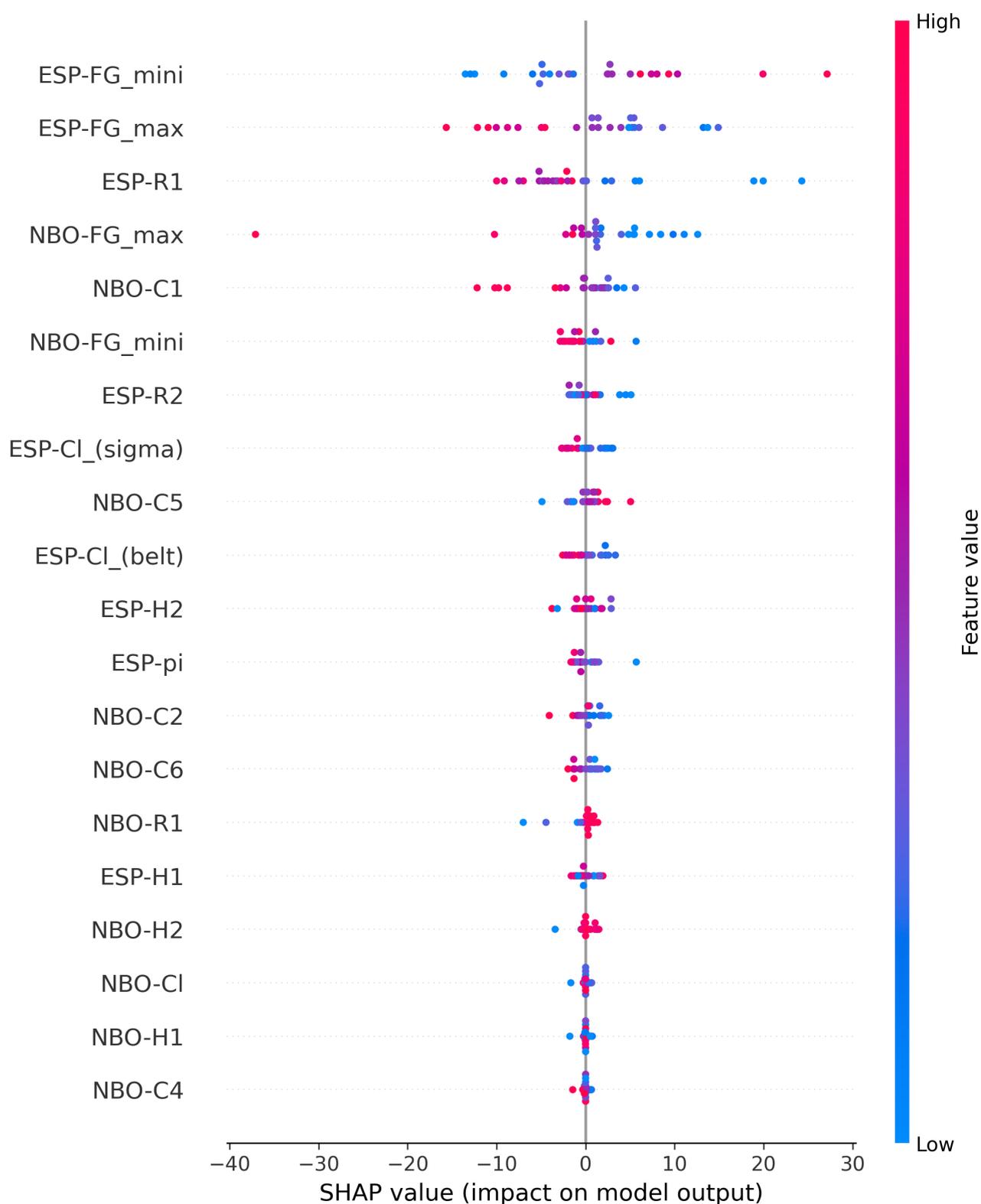


Figure S9. SHAP beeswarm plot for all descriptors. This plot displays the SHAP values of all descriptors used in the model, indicating their impact on the predicted reaction yield.

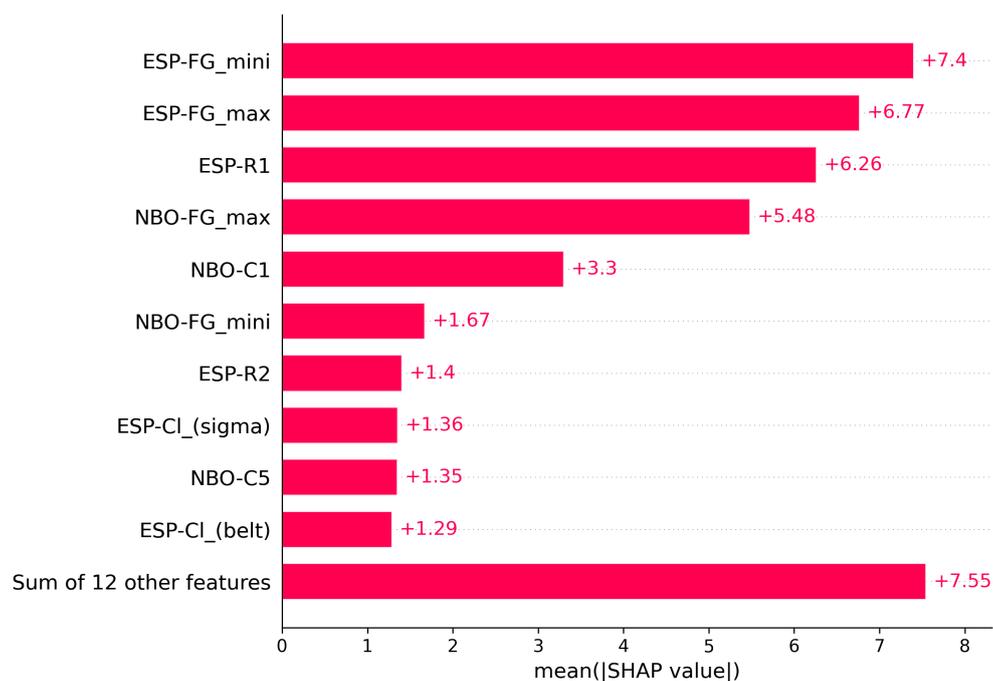
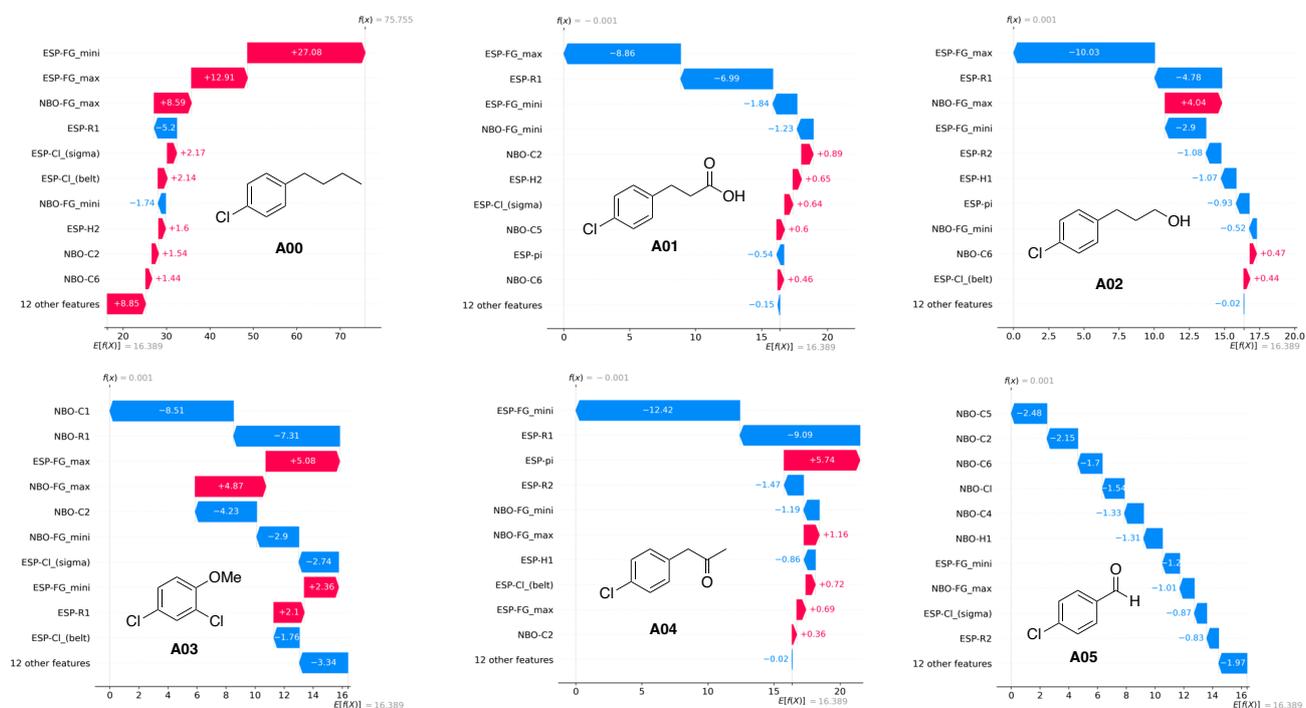
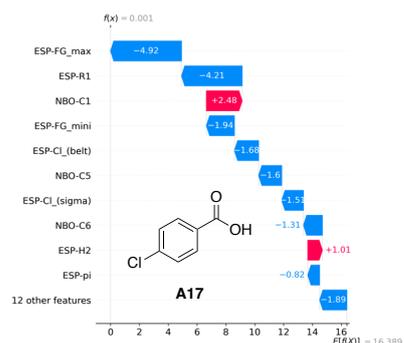
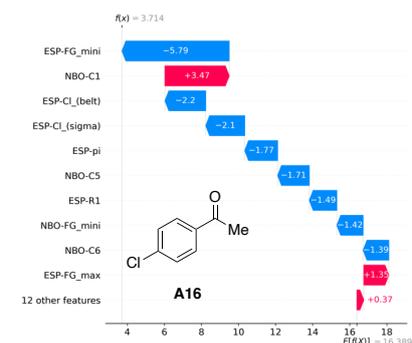
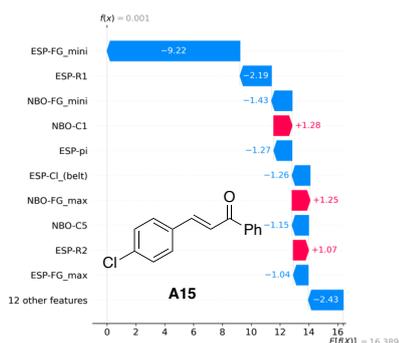
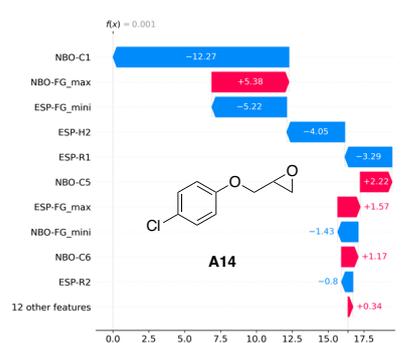
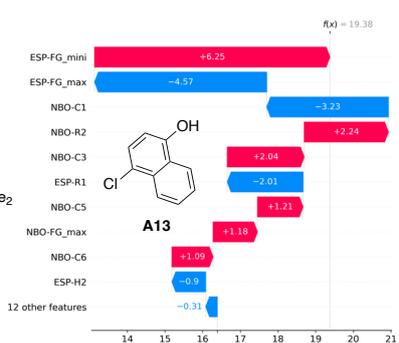
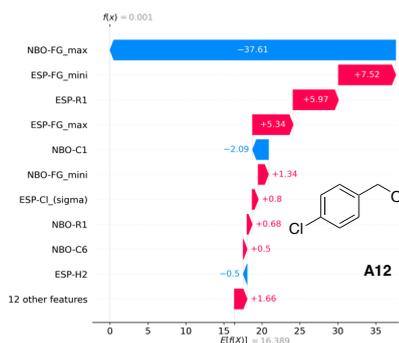
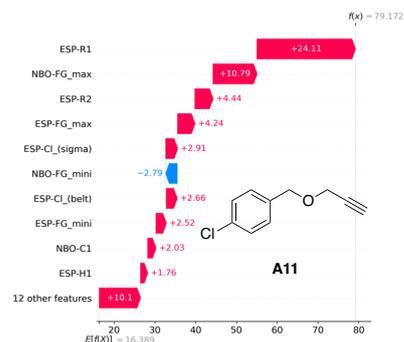
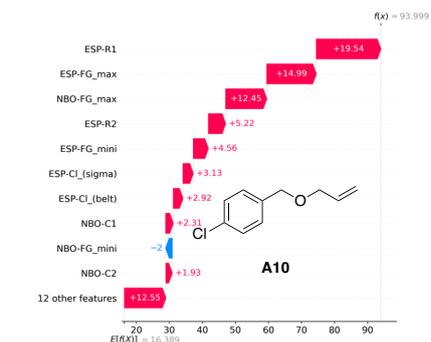
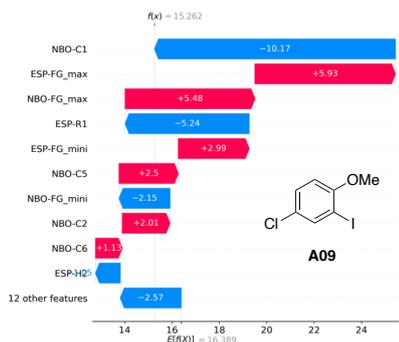
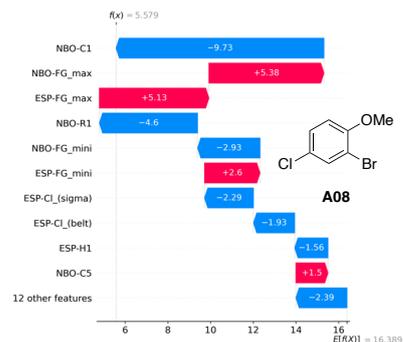
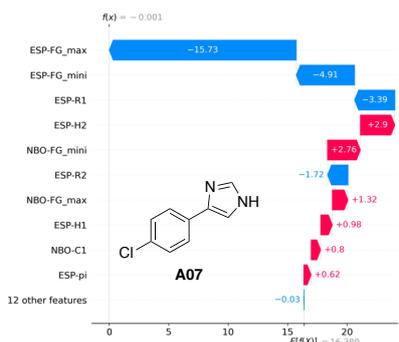
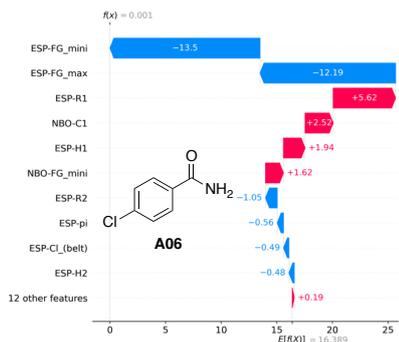


Figure S10. Bar plot of mean absolute SHAP values for the top 10 features. The plot shows the top 10 molecular descriptors ranked by their mean absolute SHAP value, indicating their relative contributions to the reaction yield prediction. The sum of the remaining 12 features is shown at the bottom.





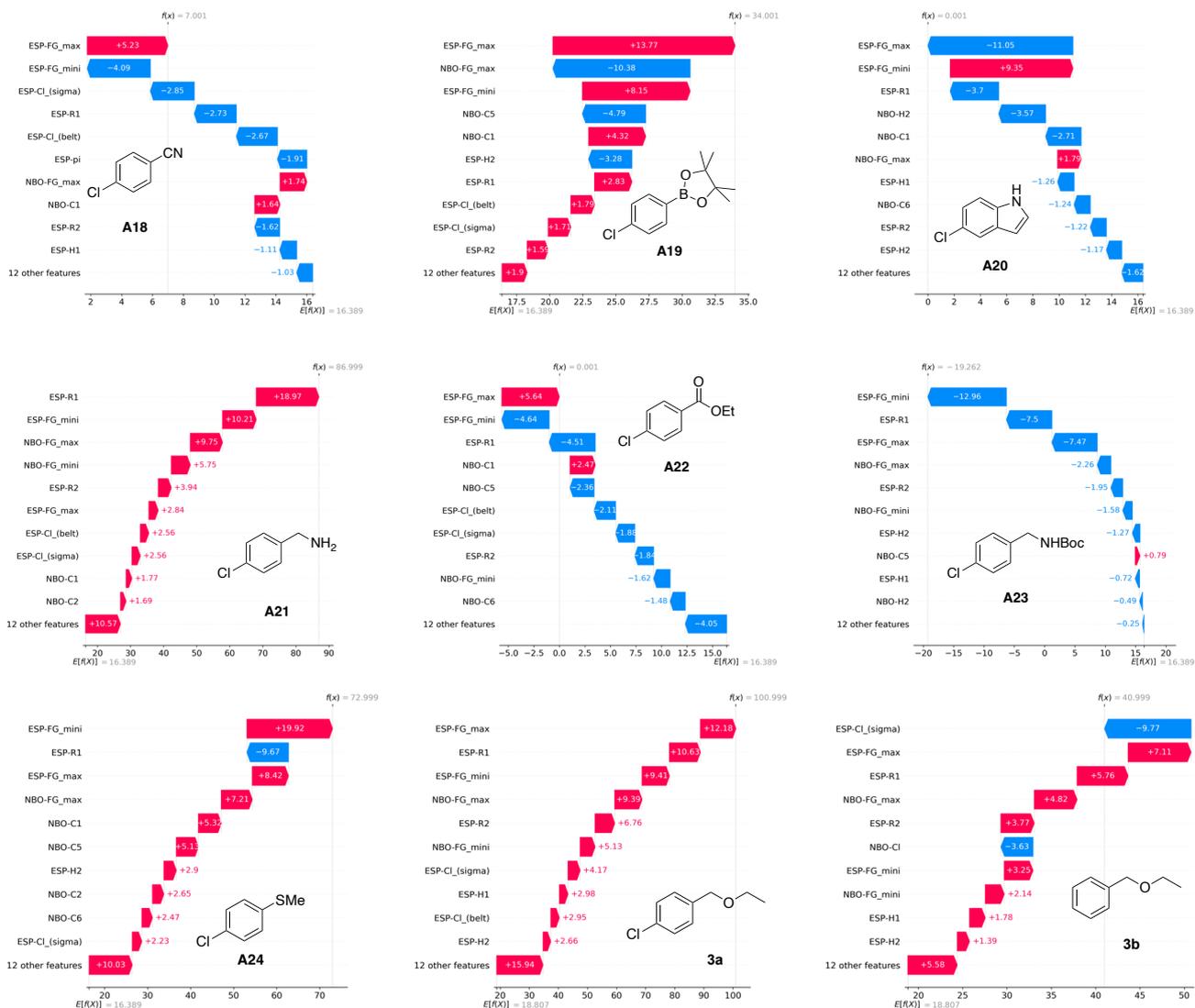


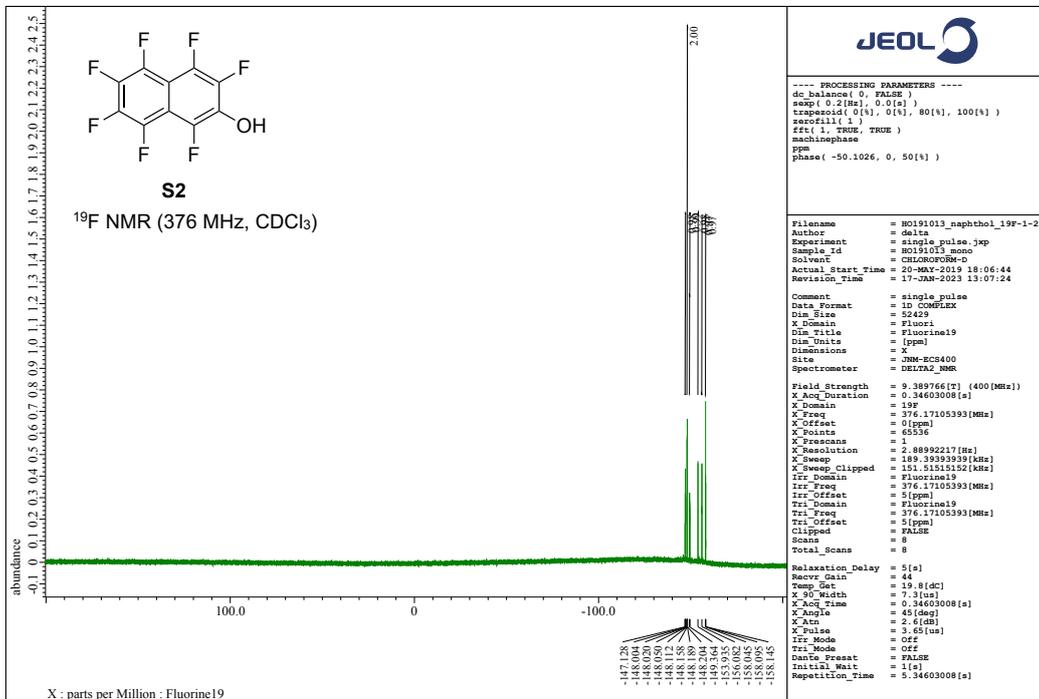
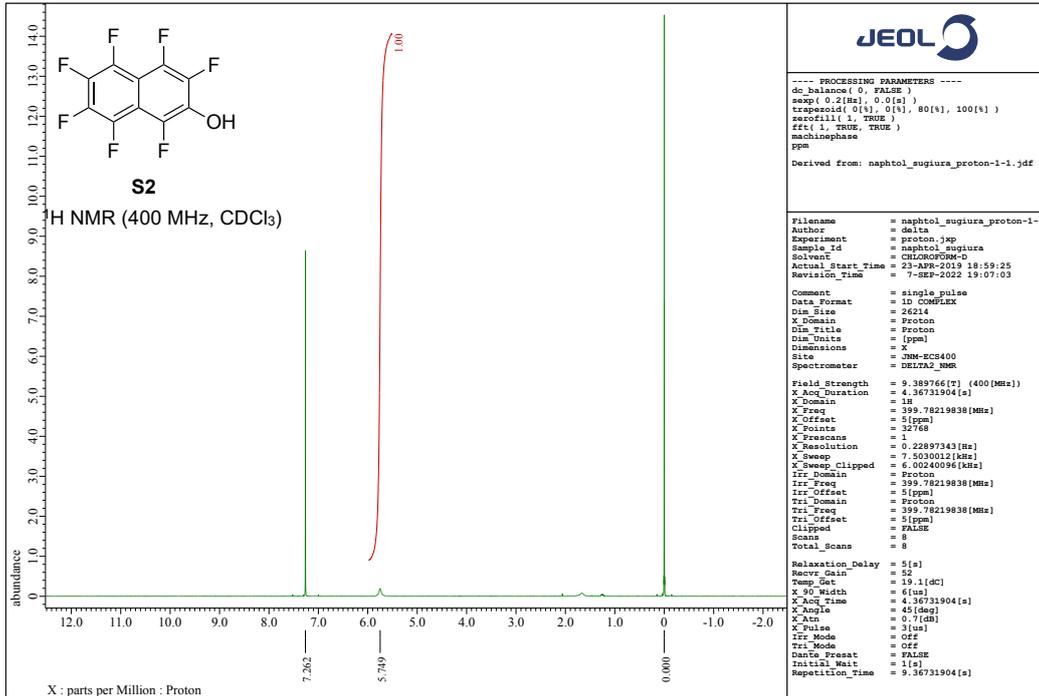
Figure S11. Waterfall plots showing SHAP values for individual additives. Each plot illustrates the contribution of descriptors to the predicted reaction yield for a given additive.

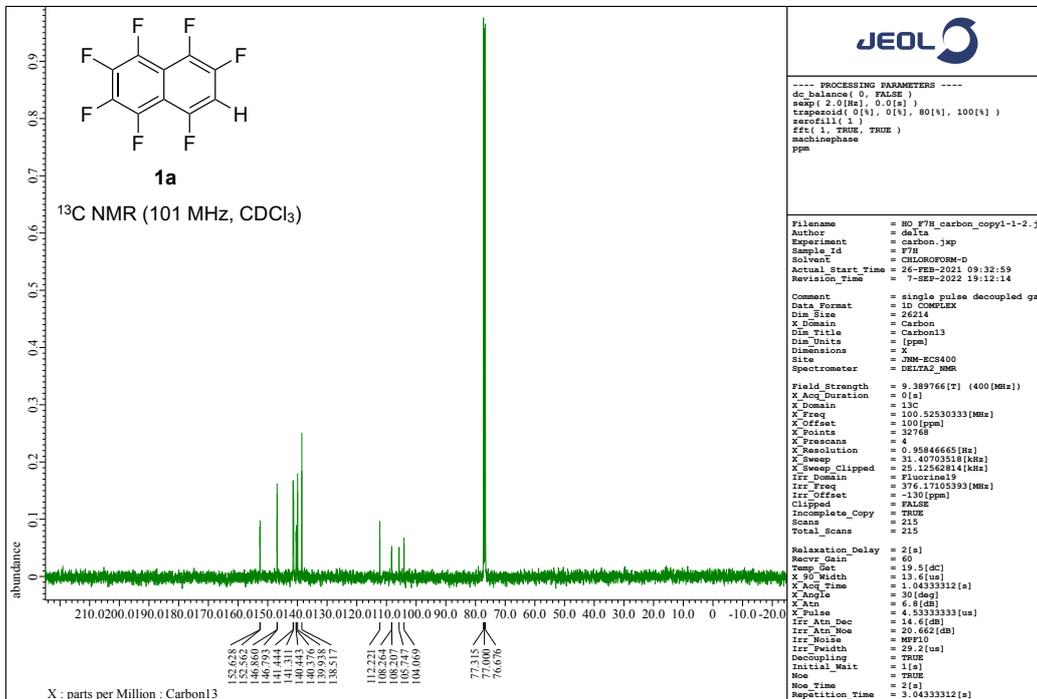
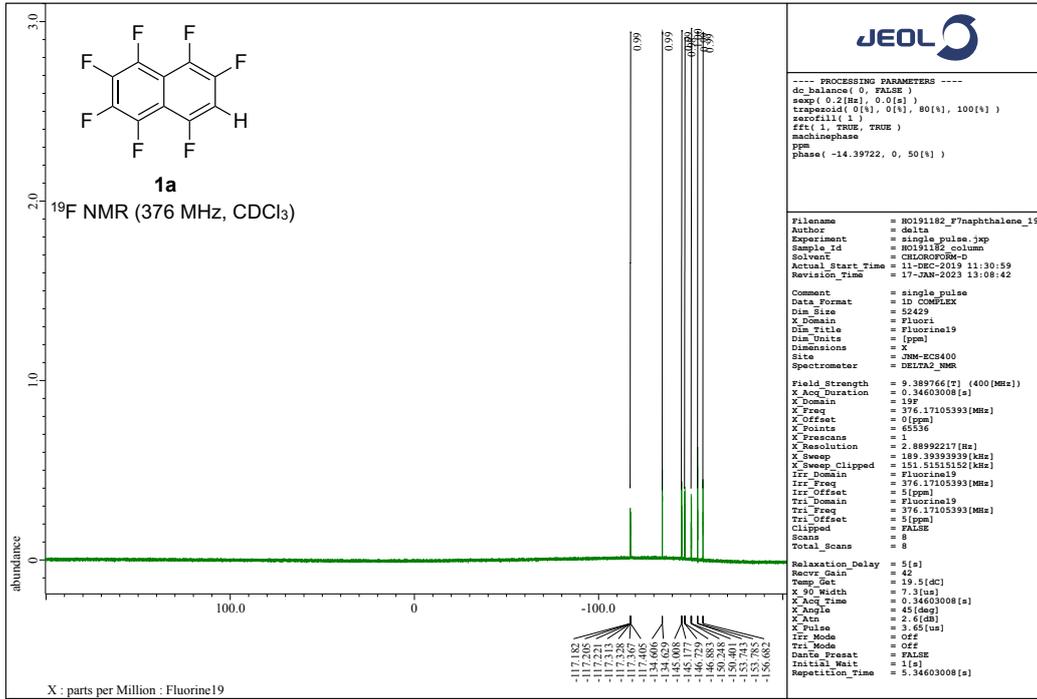
7. References

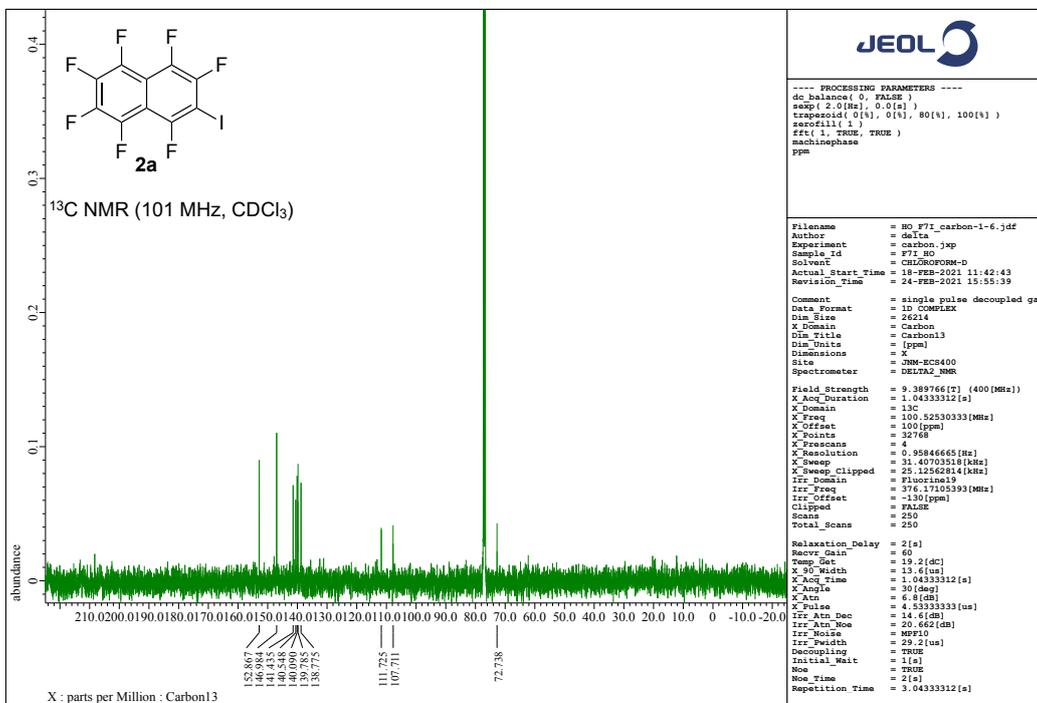
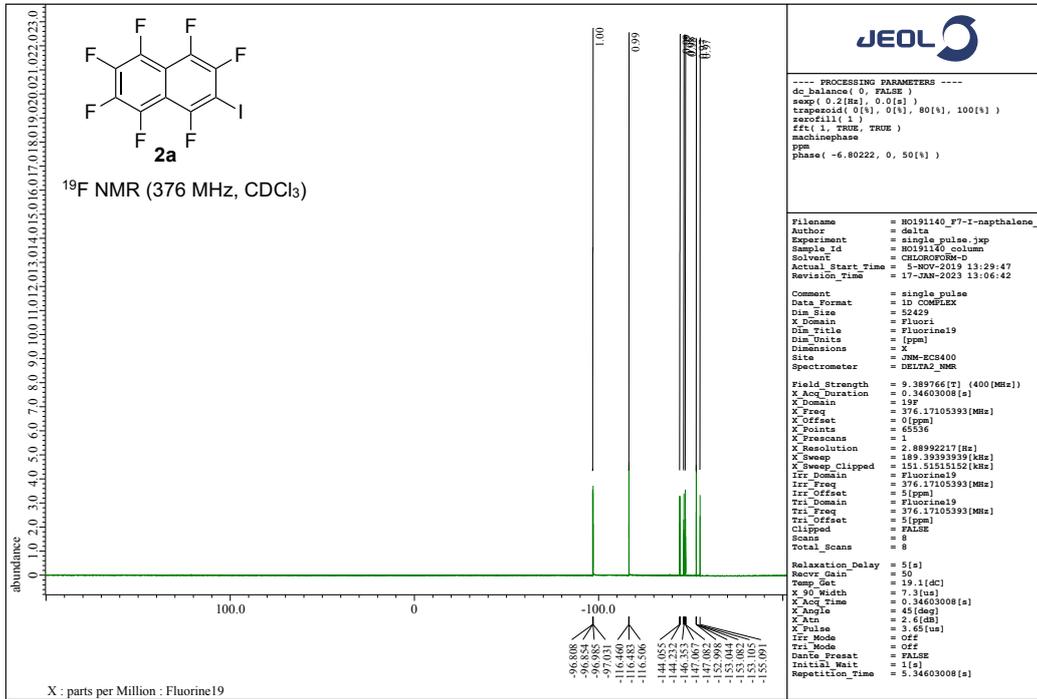
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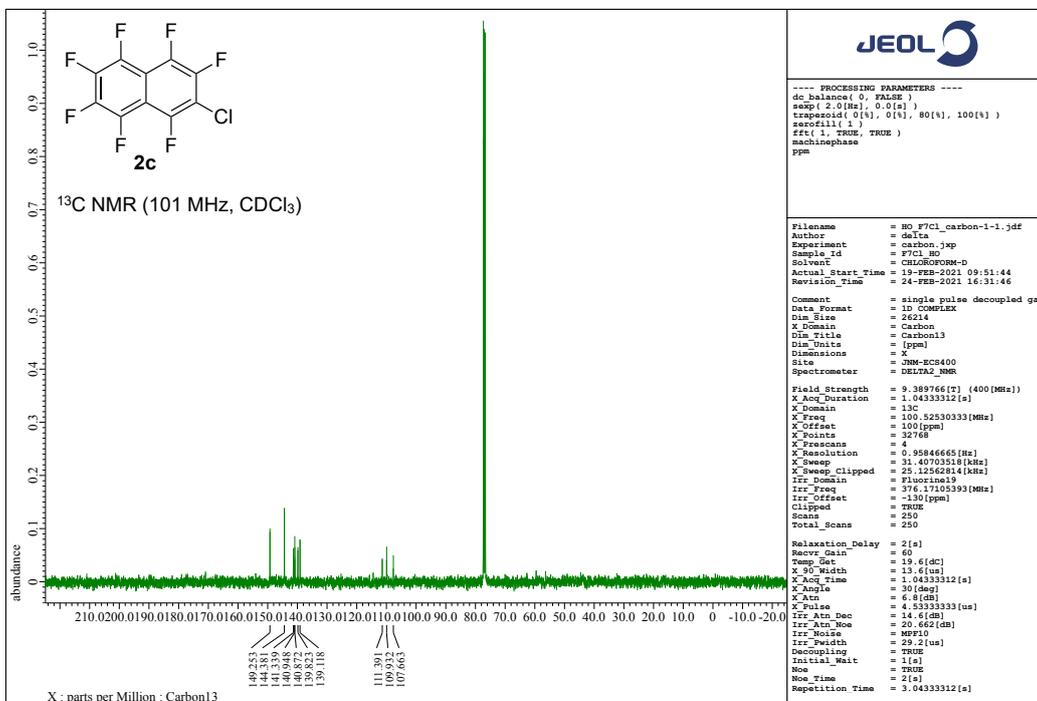
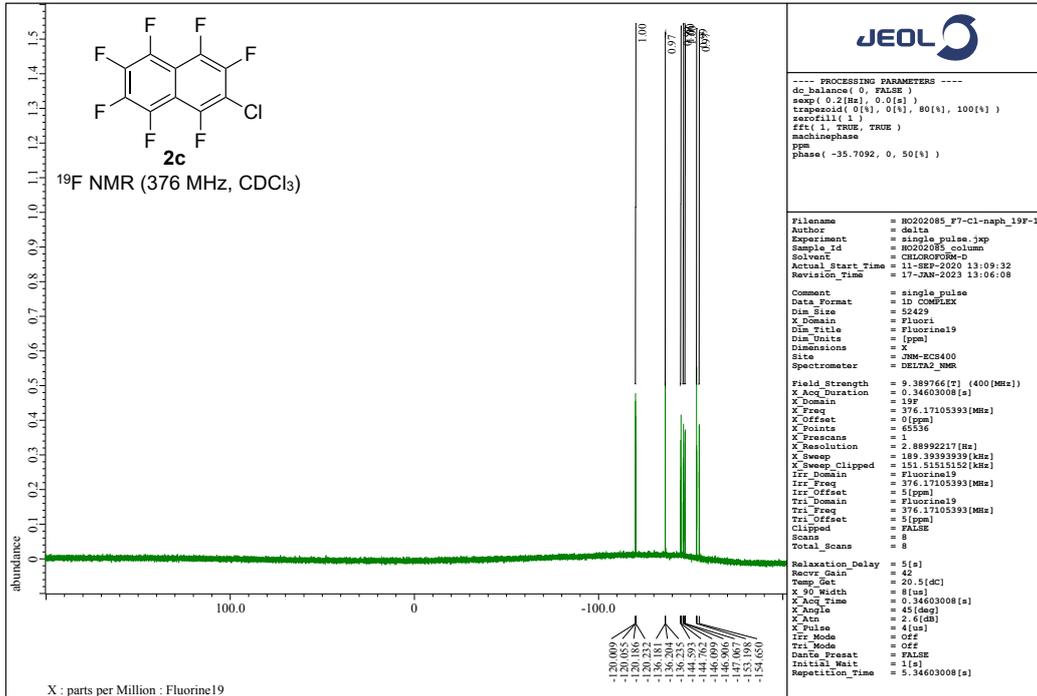
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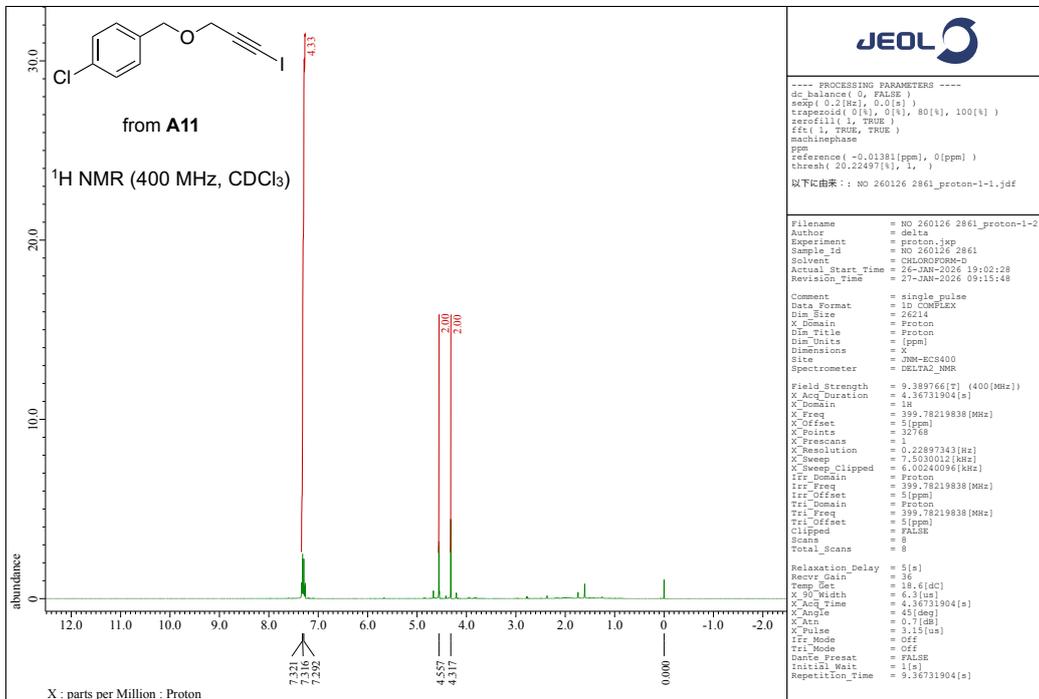
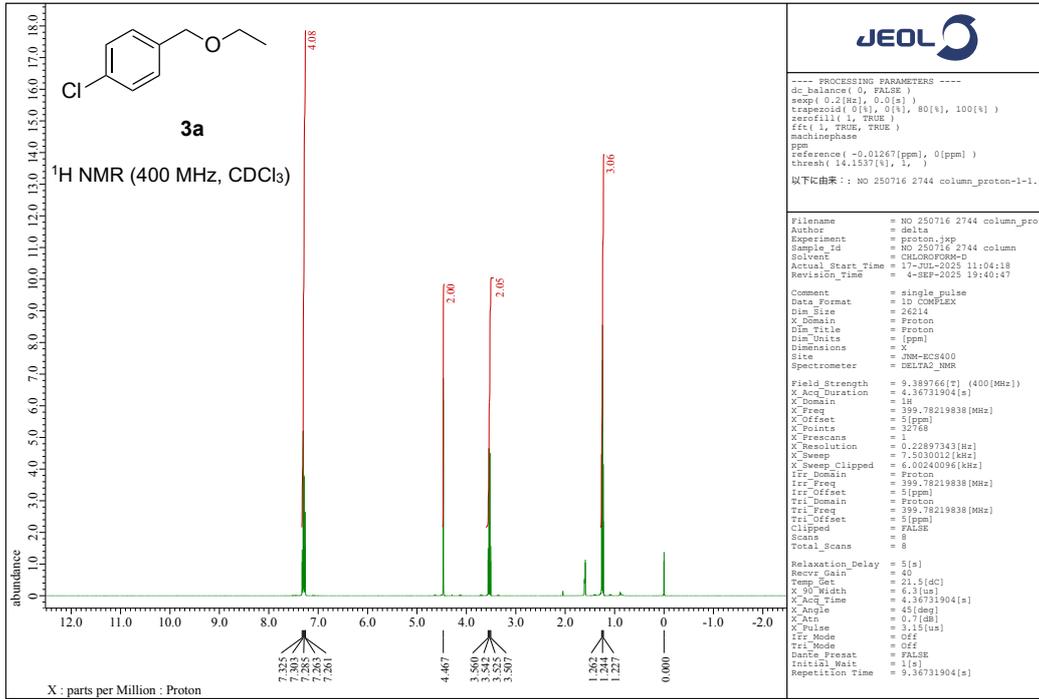
[S11] (a) M. M. Mukaka, Statistics Corner: A guide to appropriate use of Correlation coefficient in medical research. *Malawi. Med. J.* 2012, **24**, 69–71. (b) P. Schober, C. Beer and L. A. Schwarte, Correlation Coefficients: Appropriate Use and Interpretation. *Anesth. Analg.* 2018, **126**, 1763–1768.

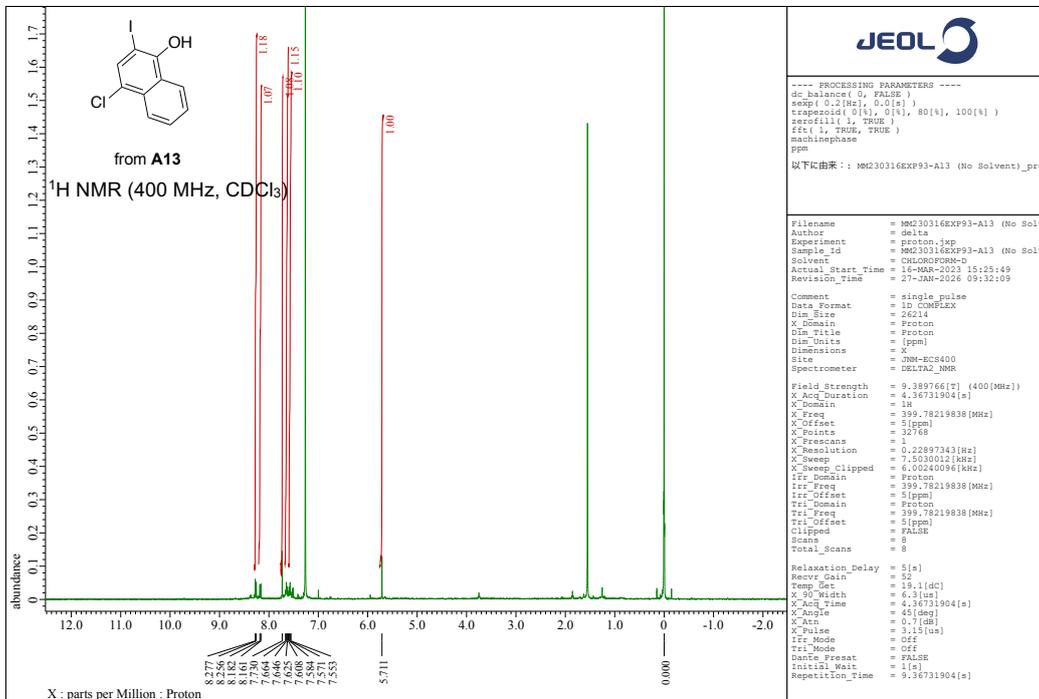
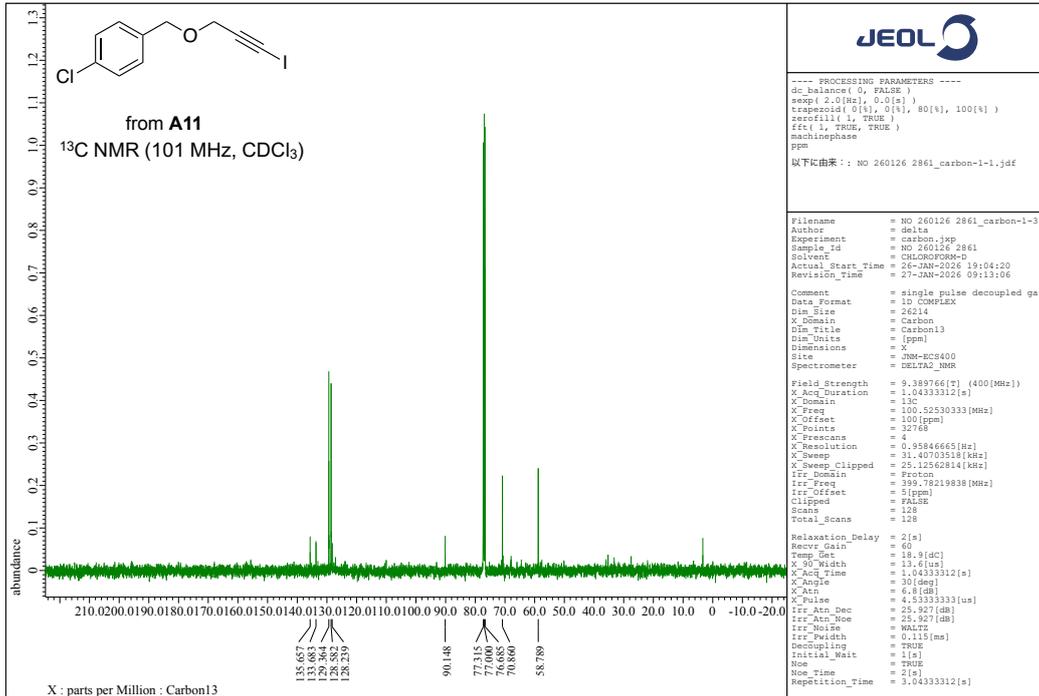


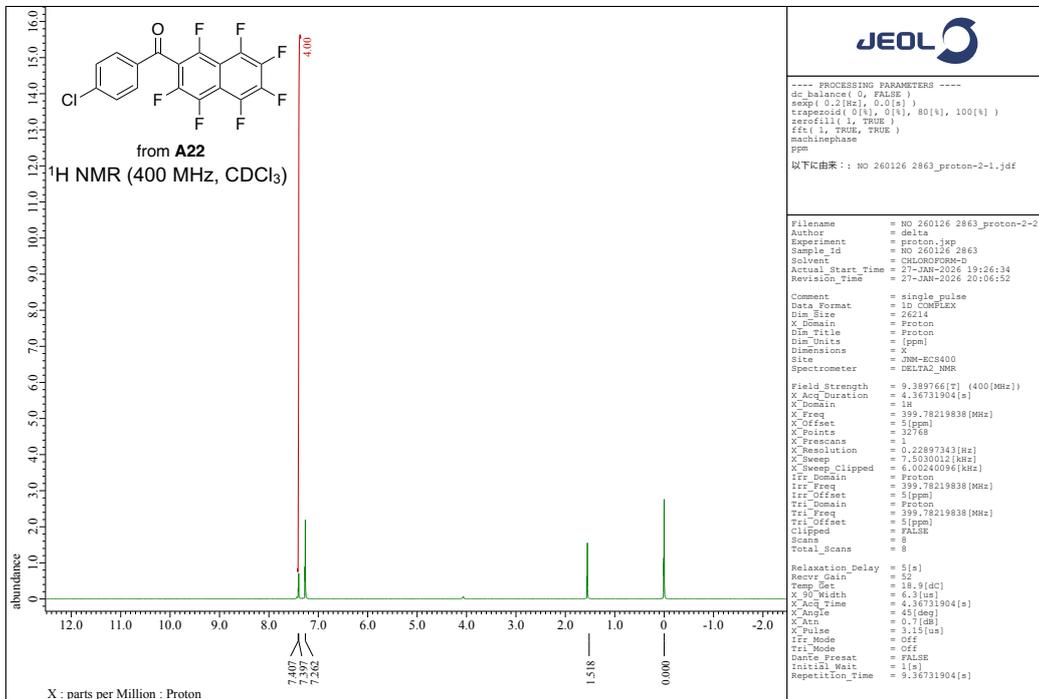
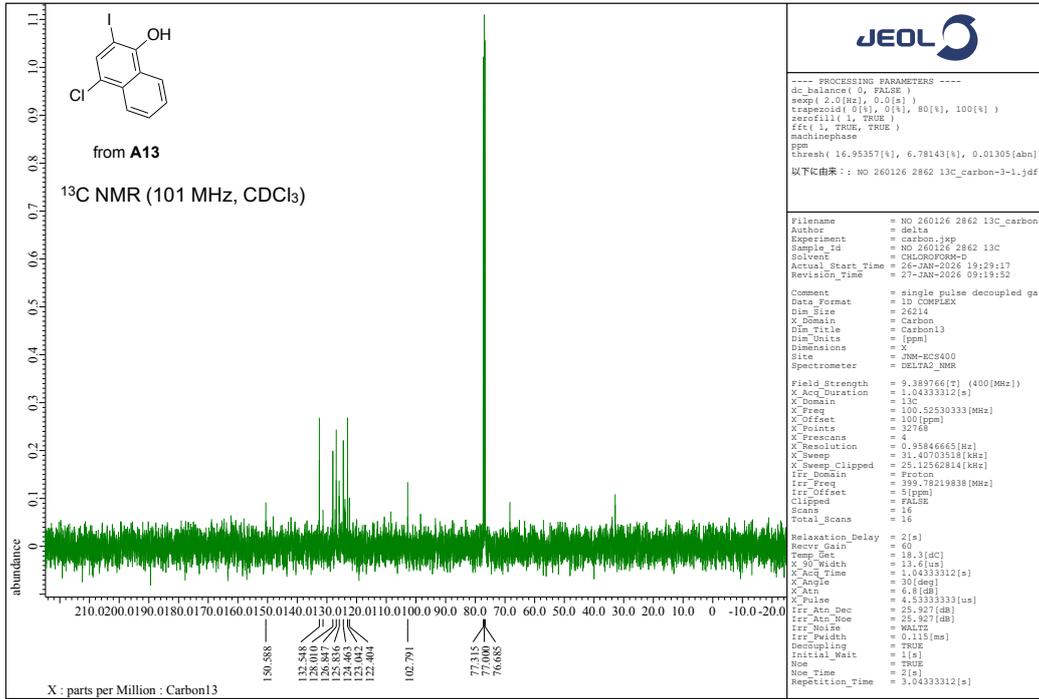


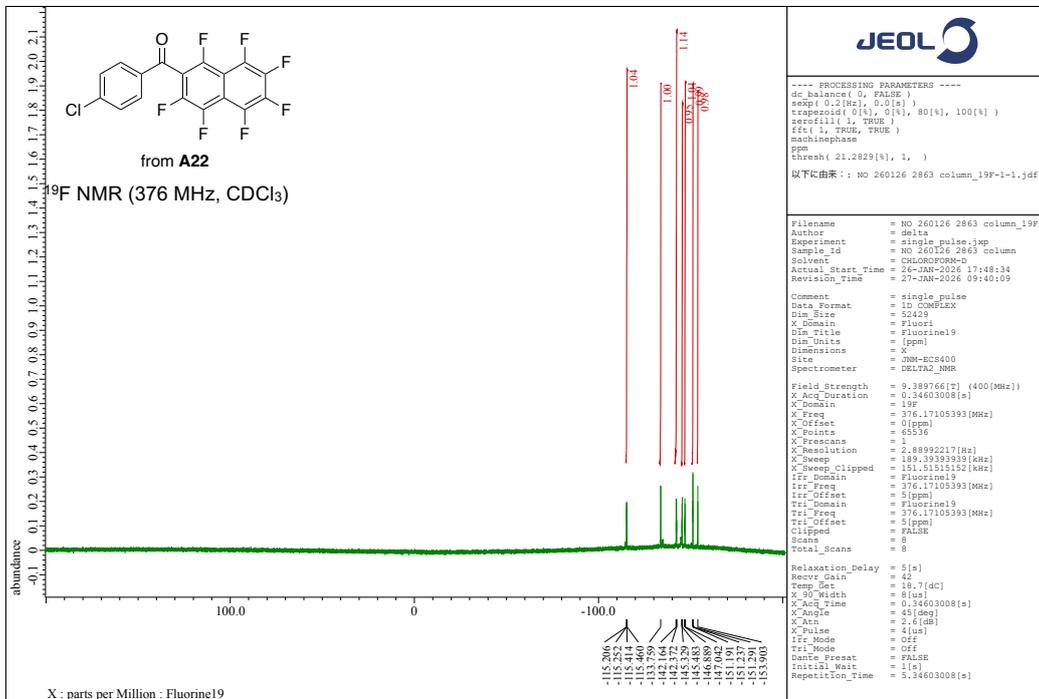
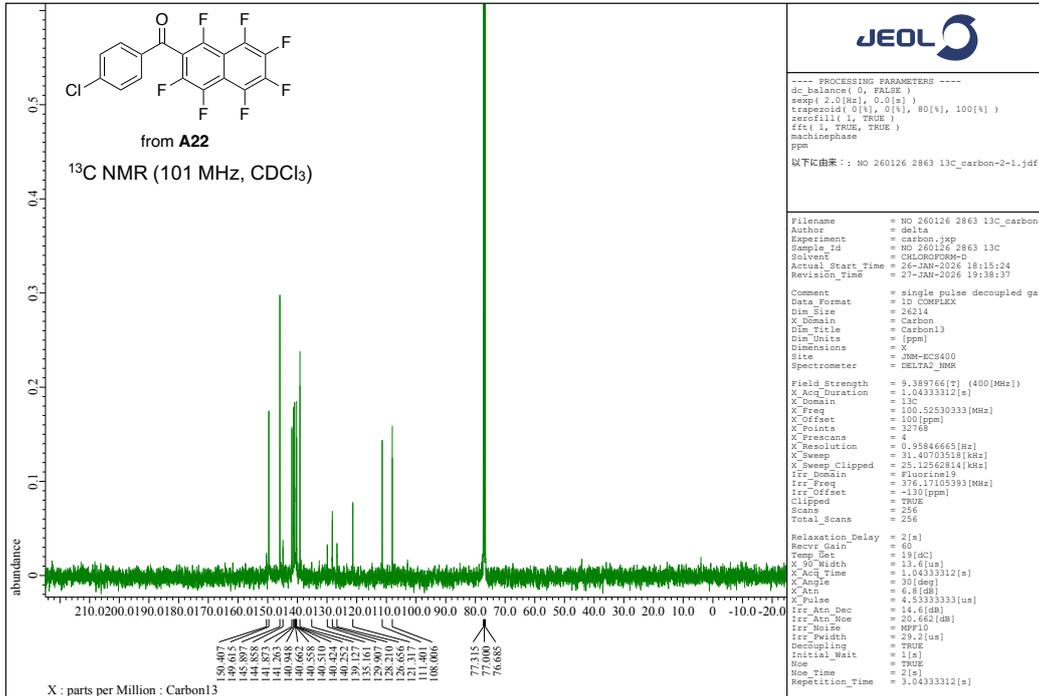












6. Cartesian coordinates

SMD(THF)/M06-2X-D3/6-311+G(d,p)
SMD18(THF)/M06-2X-D3/6-311+G(d,p)-SDD(iodine)

A00	C	-2.084569	1.228869	-0.000322
	C	-2.472462	-0.105785	-0.000013
	C	-1.536792	-1.126339	0.000350
	C	-0.180708	-0.801458	0.000425
	C	0.245988	0.526181	0.000142
	C	-0.729638	1.529956	-0.000249
	Cl	-4.180331	-0.502623	-0.000079
	C	1.707351	0.921290	0.000303
	C	2.710305	-0.227373	-0.000002
	C	4.154221	0.270238	-0.000079
	H	-2.828863	2.015998	-0.000621
	H	-1.855872	-2.161446	0.000579
	H	0.541513	-1.608975	0.000712
	H	-0.421243	2.570859	-0.000495
	H	1.889969	1.557162	-0.873698
	H	1.889919	1.556626	0.874708
	H	2.549063	-0.861808	0.879291
	H	2.548851	-0.861516	-0.879469
	H	4.316553	0.904874	-0.878113
	H	4.316719	0.904665	0.878076
	C	5.162745	-0.874718	-0.000309
	H	5.034990	-1.506745	-0.883795
	H	6.190213	-0.503316	-0.000372
	H	5.035168	-1.506943	0.883063
A01	C	2.278409	1.243537	-0.000043
	C	2.745094	-0.065908	-0.000023
	C	1.871977	-1.140282	0.000015
	C	0.498696	-0.897228	0.000035
	C	-0.004463	0.403135	0.000016
	C	0.908694	1.463828	-0.000024
	Cl	4.473077	-0.359382	-0.000050

	C	-1.482318	0.726203	0.000043
	C	-2.401829	-0.483913	0.000018
	H	2.974323	2.073572	-0.000075
	H	2.251241	-2.154842	0.000030
	H	-0.170937	-1.749261	0.000064
	H	0.537920	2.484024	-0.000040
	H	-1.704632	1.346835	0.872900
	H	-1.704652	1.346887	-0.872772
	H	-2.236807	-1.118310	-0.876545
	H	-2.236808	-1.118347	0.876555
	O	-4.657735	-1.168195	-0.000019
	H	-5.576569	-0.858005	-0.000016
	C	-3.853630	-0.091548	0.000030
	O	-4.284661	1.031945	0.000061
A02	C	2.053912	1.234998	-0.000028
	C	2.455910	-0.095422	-0.000012
	C	1.531193	-1.125978	0.000016
	C	0.171756	-0.815877	0.000029
	C	-0.268075	0.507182	0.000014
	C	0.695949	1.521752	-0.000015
	Cl	4.167668	-0.473983	-0.000028
	C	-1.732727	0.888618	0.000031
	C	-2.715425	-0.276677	0.000012
	C	-4.148628	0.216158	0.000014
	H	2.789638	2.030091	-0.000050
	H	1.861043	-2.157674	0.000028
	H	-0.541520	-1.631440	0.000050
	H	0.376299	2.559183	-0.000028
	H	-1.920917	1.521426	0.874766
	H	-1.920927	1.521463	-0.874674
	H	-2.561261	-0.905731	-0.882369
	H	-2.561268	-0.905756	0.882377
	H	-4.331912	0.834326	0.887537
	H	-4.331903	0.834362	-0.887486
	O	-5.006607	-0.919802	-0.000014

	H	-5.917969	-0.612644	0.000063
A03	C	-1.302172	-1.456571	-0.171940
	C	-1.721176	-0.144862	0.003554
	C	-0.821189	0.910478	0.036005
	C	0.530685	0.630148	-0.109985
	C	0.985360	-0.678221	-0.289450
	C	0.054794	-1.712720	-0.317122
	Cl	-3.425212	0.195609	0.184979
	C	3.008255	-1.198048	0.749962
	H	-2.022955	-2.263950	-0.198733
	H	-1.159351	1.930227	0.168460
	H	0.412067	-2.725775	-0.462562
	H	2.936520	-0.342396	1.427163
	H	2.603967	-2.089023	1.238815
	O	2.308606	-0.938598	-0.471321
	H	4.049800	-1.366224	0.482015
	Cl	1.678375	1.937608	-0.084433
A04	C	-1.489951	1.235881	-0.186137
	C	-2.115782	0.014160	0.011692
	C	-1.416359	-1.094487	0.470202
	C	-0.057928	-0.966741	0.733892
	C	0.601850	0.248719	0.546246
	C	-0.128763	1.342178	0.083770
	Cl	-3.830209	-0.133725	-0.319900
	C	2.075572	0.365495	0.808904
	C	4.424737	0.114240	-0.170869
	H	-2.053284	2.089504	-0.542615
	H	-1.924632	-2.039374	0.618097
	H	0.495459	-1.828603	1.091874
	H	0.367620	2.294978	-0.067915
	H	2.366920	1.406056	0.980249
	H	2.355826	-0.183040	1.715815
	H	4.584949	1.172449	-0.400020
	H	4.759503	-0.050784	0.855642

	C	2.955162	-0.186443	-0.307605
	O	2.508332	-0.816307	-1.236272
	H	5.003321	-0.495425	-0.863209
A05	C	-0.550498	-1.172489	0.000051
	C	-1.317669	-0.009602	-0.000066
	C	-0.744165	1.254765	0.000056
	C	0.641984	1.352401	0.000297
	C	1.429638	0.202858	0.000430
	C	0.829985	-1.058990	0.000297
	Cl	-3.057855	-0.148509	-0.000377
	H	-1.031060	-2.142671	-0.000046
	H	-1.367455	2.139942	-0.000040
	H	1.114519	2.329214	0.000398
	H	1.452008	-1.946571	0.000402
	C	2.903520	0.342204	0.000752
	H	3.273398	1.383428	-0.000617
	O	3.673170	-0.588198	-0.000575
A06	C	-1.019516	-1.207091	0.144981
	C	-1.681401	0.005996	0.001366
	C	-0.991792	1.200253	-0.158488
	C	0.397937	1.176278	-0.163914
	C	1.085407	-0.028811	-0.016489
	C	0.368356	-1.216197	0.127048
	Cl	-3.428982	0.028558	0.015428
	H	-1.579489	-2.125940	0.265733
	H	-1.529578	2.131731	-0.282650
	H	0.932367	2.108148	-0.309454
	H	0.907772	-2.150195	0.227547
	C	2.586624	-0.116577	-0.031404
	O	3.155333	-1.156776	-0.321037
	N	3.255311	1.018668	0.279848
	H	2.794827	1.813407	0.695469
	H	4.263267	0.977775	0.331843

A07	C	1.697572	1.214241	-0.025790
	C	2.366530	-0.003043	0.000133
	C	1.674949	-1.205866	0.021881
	C	0.285235	-1.185665	0.019422
	C	-0.416570	0.023026	-0.004236
	C	0.309425	1.218927	-0.029341
	C	-1.886014	0.027059	-0.001741
	C	-2.741456	1.103174	0.039902
	N	-4.000151	0.567459	0.024009
	C	-3.875459	-0.780842	-0.024143
	N	-2.615733	-1.142262	-0.039747
	H	2.252910	2.143766	-0.045002
	H	2.212601	-2.145857	0.041266
	H	-0.264802	-2.118604	0.037313
	H	-0.210401	2.170213	-0.054497
	H	-2.572532	2.166376	0.081637
	H	-4.868448	1.085616	0.046270
	H	-4.729035	-1.440203	-0.045810
	Cl	4.117978	-0.017868	0.004263
A08	C	1.955416	1.422367	-0.188200
	C	2.090381	0.053336	-0.000290
	C	0.988661	-0.788737	0.046994
	C	-0.275990	-0.231096	-0.095023
	C	-0.445991	1.141286	-0.287196
	C	0.682568	1.956671	-0.331159
	Cl	3.686812	-0.633655	0.181586
	C	-2.249419	2.217109	0.730739
	H	2.830017	2.059253	-0.227378
	H	1.111305	-1.854432	0.191459
	H	0.547749	3.020911	-0.489002
	H	-2.340255	1.445172	1.500578
	H	-1.634034	3.039642	1.106024
	O	-1.685540	1.672690	-0.465889
	H	-3.238033	2.588781	0.467377
	Br	-1.798342	-1.358123	-0.033260

A09	C	2.554215	1.223753	-0.191224
	C	2.437751	-0.146575	-0.000304
	C	1.200771	-0.774389	0.051049
	C	0.057728	0.003475	-0.090484
	C	0.142123	1.381766	-0.287082
	C	1.399854	1.980287	-0.333953
	Cl	3.882473	-1.113801	0.177872
	C	-1.410639	2.803247	0.722940
	H	3.529910	1.691146	-0.233445
	H	1.135882	-1.844864	0.198589
	H	1.460209	3.050915	-0.494297
	H	-1.621679	2.080997	1.517314
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	O	-0.979799	2.132590	-0.464993
	H	-2.321897	3.339539	0.464076
	I	-1.848812	-0.920465	-0.019713
A10	C	2.473409	1.181227	0.055008
	C	2.751313	-0.180122	0.019298
	C	1.738295	-1.124580	-0.024689
	C	0.412735	-0.695164	-0.032671
	C	0.106542	0.662194	0.001976
	C	1.147299	1.592104	0.045068
	Cl	4.421484	-0.712068	0.028910
	C	-1.316498	1.158082	0.002106
	C	-3.561685	0.503195	-0.120455
	H	3.279024	1.904411	0.088434
	H	1.976409	-2.180886	-0.052179
	H	-0.387476	-1.423400	-0.067039
	H	0.920180	2.653426	0.071068
	H	-1.513177	1.703735	0.936375
	H	-1.458307	1.867647	-0.825571
	H	-3.808193	0.981772	0.836309
	H	-3.711332	1.243671	-0.919987
	O	-2.208949	0.078123	-0.125636

	C	-4.438204	-0.685495	-0.356344
	H	-4.213111	-1.269574	-1.245803
	C	-5.449193	-1.023393	0.435342
	H	-5.680826	-0.452165	1.329950
	H	-6.080908	-1.876748	0.214215
A11	C	2.363777	1.173557	-0.000139
	C	2.622045	-0.192093	-0.000009
	C	1.595442	-1.122792	0.000166
	C	0.275980	-0.675101	0.000222
	C	-0.009864	0.686975	0.000100
	C	1.043671	1.603196	-0.000093
	Cl	4.284195	-0.747399	-0.000073
	C	-1.424337	1.205368	0.000231
	C	-3.671238	0.578180	0.000009
	H	3.179788	1.885733	-0.000287
	H	1.818162	-2.182798	0.000253
	H	-0.533751	-1.393572	0.000356
	H	0.831601	2.667906	-0.000207
	H	-1.586398	1.834736	0.886485
	H	-1.586339	1.835374	-0.885579
	H	-3.869632	1.193670	0.887009
	H	-3.869775	1.193959	-0.886759
	O	-2.332746	0.126027	-0.000169
	C	-4.569837	-0.576001	-0.000093
	C	-5.320333	-1.512779	-0.000149
	H	-5.984836	-2.348502	-0.000151
A12	C	3.594501	1.113968	0.119735
	C	3.684834	-0.266038	-0.010783
	C	2.601485	-1.027573	-0.423016
	C	1.398716	-0.387785	-0.710240
	C	1.278317	0.993762	-0.584410
	C	2.384712	1.734744	-0.167455
	C	-0.021157	1.700407	-0.909303
	C	-3.170193	-0.958321	-0.159748

C	-2.308527	-2.061008	-0.790373
C	-3.902860	-1.526035	1.064685
C	-4.199933	-0.468047	-1.186976
O	-1.118283	0.817372	-0.964168
Si	-2.069741	0.475365	0.380947
C	-3.065999	2.001304	0.813259
C	-0.986377	0.011373	1.837624
H	4.450917	1.690242	0.447776
H	2.693171	-2.102761	-0.517870
H	0.542000	-0.970413	-1.028565
H	2.302334	2.811795	-0.058265
H	-0.183652	2.503419	-0.177571
H	0.069747	2.180465	-1.889155
H	-1.802473	-1.704262	-1.691494
H	-1.546952	-2.430613	-0.095432
H	-2.938557	-2.914057	-1.071587
H	-4.580446	-2.331280	0.755538
H	-4.507104	-0.765661	1.570839
H	-3.204499	-1.944887	1.796007
H	-4.878456	0.274113	-0.755100
H	-3.716951	-0.018307	-2.060060
H	-4.809977	-1.309037	-1.539279
H	-2.422851	2.792304	1.211333
H	-3.584955	2.398094	-0.063585
H	-3.815353	1.776276	1.578723
H	-0.479325	-0.946366	1.691340
H	-0.219474	0.772606	2.015108
H	-1.591360	-0.060004	2.747328
Cl	5.201279	-1.062368	0.362120
A13			
C	0.099502	-2.321489	0.000006
C	-1.196040	-1.761035	0.000002
C	-1.360064	-0.405526	-0.000007
C	-0.246301	0.481523	-0.000007
C	1.058550	-0.087837	0.000009
C	1.201383	-1.506871	0.000011

	C	-0.367742	1.895020	-0.000015
	C	0.746982	2.693341	-0.000008
	C	2.040010	2.124934	0.000010
	C	2.192001	0.762771	0.000017
	O	2.471998	-1.982007	0.000005
	Cl	-2.986559	0.245195	-0.000019
	H	0.216158	-3.399724	0.000004
	H	-2.060227	-2.413708	0.000002
	H	-1.353322	2.342328	-0.000027
	H	0.634990	3.771276	-0.000016
	H	2.911232	2.769213	0.000018
	H	3.178320	0.316358	0.000032
	H	2.458669	-2.946989	0.000169
A14	C	1.854799	-1.146632	-0.014640
	C	2.690633	-0.045299	0.035166
	C	2.177102	1.247726	-0.001275
	C	0.807713	1.429436	-0.089293
	C	-0.051091	0.326595	-0.141073
	C	0.474909	-0.964564	-0.103018
	O	-1.373778	0.610417	-0.227137
	C	-3.661995	0.097168	-0.409619
	C	-4.807639	-0.643611	0.123794
	O	-4.276061	0.483734	0.812338
	Cl	4.424159	-0.278307	0.146132
	C	-2.285927	-0.478721	-0.304179
	H	2.265754	-2.148309	0.015511
	H	2.841418	2.102250	0.038368
	H	0.383148	2.425815	-0.118554
	H	-0.164313	-1.836560	-0.139497
	H	-3.822638	0.789490	-1.231657
	H	-5.786256	-0.496914	-0.320627
	H	-4.640719	-1.599565	0.611451
	H	-2.068357	-1.088017	-1.189062
	H	-2.211046	-1.102771	0.593055

A15	C	3.320097	-1.175813	-0.373381
	C	4.329694	-0.283464	-0.025481
	C	4.048966	1.023366	0.345310
	C	2.723586	1.439696	0.366073
	C	1.683010	0.567332	0.028112
	C	2.003221	-0.745473	-0.345011
	C	0.306523	1.068434	0.075867
	Cl	5.990901	-0.824011	-0.062029
	C	-0.813388	0.355353	-0.100320
	C	-2.137473	1.025383	-0.035258
	C	-3.364490	0.165118	-0.002115
	O	-2.240422	2.238323	-0.022510
	C	-3.331892	-1.165235	0.423983
	C	-4.504947	-1.912582	0.469529
	C	-5.710980	-1.342314	0.074188
	C	-5.748631	-0.016202	-0.354578
	C	-4.582591	0.735986	-0.383411
	H	3.564986	-2.189688	-0.664539
	H	4.848988	1.703104	0.610565
	H	2.490689	2.459669	0.652289
	H	1.221405	-1.441625	-0.624316
	H	0.199487	2.130294	0.285806
	H	-0.785350	-0.708729	-0.298982
	H	-2.402280	-1.619112	0.746369
	H	-4.475800	-2.939674	0.813845
	H	-6.622077	-1.929139	0.101299
	H	-6.687555	0.428575	-0.663125
	H	-4.598671	1.770423	-0.705669
A16	C	-0.980290	-1.206250	-0.000136
	C	-1.692947	-0.015480	-0.000009
	C	-1.056140	1.220997	0.000055
	C	0.329889	1.255700	-0.000013
	C	1.074538	0.073533	-0.000142
	C	0.409105	-1.153802	-0.000193
	C	2.574030	0.165844	-0.000217

	Cl	-3.439365	-0.069522	0.000078
	C	3.370075	-1.111807	0.000249
	O	3.117066	1.249891	0.000045
	H	-1.499367	-2.156415	-0.000187
	H	-1.636568	2.135065	0.000154
	H	0.848454	2.206833	0.000030
	H	0.963935	-2.084110	-0.000288
	H	3.127277	-1.709406	0.882666
	H	3.127887	-1.709613	-0.882198
	H	4.431501	-0.872027	0.000576
A17	C	-0.984100	-1.208861	-0.000024
	C	-1.675354	-0.003758	0.000044
	C	-1.018480	1.221529	0.000056
	C	0.368429	1.233297	-0.000005
	C	1.082194	0.034986	-0.000077
	C	0.404316	-1.184390	-0.000082
	C	2.568126	0.105150	-0.000155
	Cl	-3.420786	-0.028060	0.000119
	O	3.149107	-1.103239	0.000005
	O	3.202733	1.129217	-0.000077
	H	-1.521349	-2.148734	-0.000032
	H	-1.582486	2.145579	0.000111
	H	0.905547	2.173954	0.000000
	H	0.956075	-2.115714	-0.000135
	H	4.110068	-0.973610	0.000054
A18	C	0.577765	1.215557	0.000000
	C	1.252290	-0.000001	0.000000
	C	0.577751	-1.215551	0.000000
	C	-0.808840	-1.214522	0.000000
	C	-1.499217	0.000017	0.000000
	C	-0.808826	1.214546	0.000000
	Cl	2.994633	-0.000012	0.000000
	C	-2.934435	0.000031	0.000000
	N	-4.084757	-0.000040	-0.000001

	H	1.127686	2.147913	0.000000
	H	1.127661	-2.147914	0.000000
	H	-1.354881	-2.149586	0.000000
	H	-1.354855	2.149617	0.000000
A19	C	-2.988702	-1.202261	0.171686
	C	-3.662761	0.000000	0.000000
	C	-2.988704	1.202262	-0.171687
	C	-1.598454	1.190026	-0.169448
	C	-0.882173	0.000003	0.000000
	C	-1.598452	-1.190022	0.169448
	B	0.674016	0.000003	0.000002
	Cl	-5.413618	-0.000001	0.000000
	O	1.426663	1.120739	-0.221903
	C	2.803331	0.776667	0.092262
	C	2.803328	-0.776668	-0.092263
	O	1.426660	-1.120736	0.221906
	C	3.728963	-1.526799	0.846974
	C	3.046475	-1.201896	-1.536365
	C	3.728966	1.526795	-0.846976
	C	3.046481	1.201893	1.536364
	H	-3.540506	-2.124874	0.303194
	H	-3.540509	2.124874	-0.303194
	H	-1.063025	2.124210	-0.301526
	H	-1.063021	-2.124205	0.301525
	H	3.671210	-2.597292	0.638148
	H	4.762566	-1.204464	0.694548
	H	3.459789	-1.363508	1.890650
	H	4.082151	-1.019163	-1.830811
	H	2.844036	-2.270986	-1.627811
	H	2.386295	-0.666442	-2.223320
	H	3.671216	2.597289	-0.638150
	H	4.762568	1.204458	-0.694552
	H	3.459789	1.363505	-1.890651
	H	4.082157	1.019158	1.830808
	H	2.844046	2.270985	1.627811

	H	2.386301	0.666441	2.223320
A20	C	0.881567	-1.111505	0.000000
	C	-0.410244	-1.666926	0.000000
	C	-1.518048	-0.840187	0.000000
	C	-1.301056	0.540204	0.000000
	C	0.000000	1.100605	0.000000
	C	1.115049	0.246579	0.000000
	N	-2.193885	1.581688	0.000000
	C	-1.506468	2.769660	0.000000
	C	-0.160296	2.526670	0.000000
	Cl	2.252861	-2.210137	0.000000
	H	-0.529598	-2.742974	0.000000
	H	-2.519424	-1.253992	0.000000
	H	2.124779	0.638876	0.000000
	H	-3.199621	1.491052	0.000000
	H	-2.041813	3.706711	0.000000
	H	0.621215	3.270241	0.000000
A21	C	-0.861032	1.251378	0.067398
	C	-1.425516	-0.013089	-0.006421
	C	-0.641127	-1.149773	-0.154633
	C	0.739585	-1.008579	-0.232415
	C	1.339102	0.250830	-0.164539
	C	0.523763	1.371342	-0.009673
	C	2.838980	0.405349	-0.284308
	Cl	-3.167286	-0.181919	0.096465
	N	3.547219	-0.661247	0.425668
	H	-1.488291	2.125819	0.190393
	H	-1.102237	-2.128511	-0.208314
	H	1.361992	-1.888781	-0.343373
	H	0.972723	2.357138	0.055603
	H	3.115332	0.337972	-1.341379
	H	3.111783	1.412649	0.053213
	H	4.544708	-0.583779	0.254025
	H	3.414788	-0.555911	1.427802

A22	C	-1.605425	-1.208255	0.000010
	C	-2.511349	-0.155171	0.000004
	C	-2.096558	1.171139	-0.000007
	C	-0.735830	1.443177	-0.000011
	C	0.191573	0.401856	-0.000005
	C	-0.246322	-0.922443	0.000006
	C	1.642532	0.752722	-0.000008
	Cl	-4.222021	-0.509019	0.000007
	O	2.059648	1.885269	-0.000009
	O	2.429422	-0.322730	-0.000004
	C	4.540984	-1.419714	0.000008
	C	3.851253	-0.077351	-0.000003
	H	-1.956542	-2.232369	0.000018
	H	-2.823948	1.973212	-0.000012
	H	-0.385262	2.468091	-0.000018
	H	0.471907	-1.732224	0.000011
	H	5.622507	-1.269947	0.000002
	H	4.272292	-1.994687	0.888185
	H	4.272284	-1.994707	-0.888153
	H	4.101706	0.509937	-0.885565
	H	4.101705	0.509953	0.885548
A23	C	3.799961	0.937511	-0.209720
	C	3.684612	-0.430755	0.003943
	C	2.462235	-1.016163	0.292584
	C	1.328477	-0.210028	0.369002
	C	1.412856	1.163393	0.160818
	C	2.658894	1.724464	-0.127702
	C	0.199515	2.075151	0.219816
	Cl	5.117203	-1.435560	-0.090188
	N	-1.002521	1.456396	0.727076
	O	-2.795751	0.161416	0.641727
	C	-3.810899	-0.679223	0.007637
	C	-4.643854	0.142882	-0.968672
	C	-4.663061	-1.125518	1.187585

	C	-3.155265	-1.882767	-0.659494
	C	-1.828378	0.744292	-0.084676
	O	-1.700706	0.668606	-1.289043
	H	4.763954	1.378376	-0.432536
	H	2.391556	-2.084563	0.455819
	H	0.374173	-0.671570	0.597109
	H	2.740587	2.794609	-0.291198
	H	0.429164	2.939368	0.845889
	H	-0.012561	2.448985	-0.784173
	H	-1.133688	1.368784	1.724513
	H	-4.061518	0.441281	-1.839120
	H	-5.493265	-0.457344	-1.303951
	H	-5.032075	1.036712	-0.473505
	H	-4.058342	-1.680923	1.908067
	H	-5.469299	-1.772643	0.836286
	H	-5.102924	-0.261296	1.690397
	H	-2.567801	-1.588999	-1.528255
	H	-2.507892	-2.402173	0.052209
	H	-3.933752	-2.578472	-0.982076
A24	C	-0.950043	-1.153876	0.000087
	C	-1.764981	-0.033912	0.000007
	C	-1.225472	1.247485	-0.000041
	C	0.152381	1.400468	-0.000026
	C	0.995680	0.282588	0.000064
	C	0.433722	-0.994244	0.000128
	Cl	-3.504596	-0.232168	-0.000044
	S	2.739362	0.596123	0.000073
	C	3.445702	-1.068080	-0.000187
	H	-1.381888	-2.147255	0.000125
	H	-1.873168	2.115594	-0.000108
	H	0.574827	2.399520	-0.000086
	H	1.055746	-1.879643	0.000204
	H	4.526472	-0.925094	-0.000414
	H	3.162408	-1.618480	0.896958
	H	3.162005	-1.618336	-0.897292

3a	C	2.023571	1.228631	-0.024452
	C	2.377950	-0.115091	-0.001387
	C	1.419763	-1.115501	0.031004
	C	0.072104	-0.761456	0.041008
	C	-0.310620	0.576595	0.019019
	C	0.676216	1.563911	-0.014945
	Cl	4.075624	-0.551934	-0.015218
	C	-1.760227	0.989231	0.036582
	C	-3.966859	0.199480	0.010892
	H	2.786788	1.996716	-0.051492
	H	1.717086	-2.156855	0.047909
	H	-0.686225	-1.533553	0.065030
	H	0.390047	2.610982	-0.034608
	H	-1.962283	1.572521	0.947020
	H	-1.963328	1.646676	-0.821199
	H	-4.191363	0.762602	0.926788
	H	-4.195416	0.848479	-0.845245
	O	-2.591022	-0.142669	-0.008967
	C	-4.780300	-1.073575	-0.049410
	H	-4.556349	-1.712592	0.807289
	H	-5.846572	-0.837822	-0.035995
	H	-4.559405	-1.626265	-0.964918
3b	C	-3.017316	-0.764109	-0.000591
	C	-3.244019	0.611803	-0.000369
	C	-2.161972	1.484914	0.000188
	C	-0.857319	0.991763	0.000528
	C	-0.626865	-0.381633	0.000306
	C	-1.717453	-1.255251	-0.000259
	C	0.767095	-0.956538	0.000761
	C	3.050897	-0.431671	-0.000130
	H	-3.854501	-1.453136	-0.001037
	H	-2.329704	2.556246	0.000358
	H	-0.014209	1.671197	0.000938
	H	-1.542740	-2.327351	-0.000443

H	0.897595	-1.596581	0.885780
H	0.897880	-1.597372	-0.883631
H	3.205083	-1.061110	0.886844
H	3.204171	-1.061390	-0.887060
O	1.726007	0.071172	0.000467
C	4.010647	0.736765	-0.000775
H	3.861546	1.355928	0.886267
H	5.041200	0.375269	-0.001204
H	3.860685	1.355638	-0.887869
H	-4.257233	0.997026	-0.000637
F7MgTMP			
C	5.389067	-0.204955	-0.128465
C	4.816756	-1.488900	-0.133352
C	3.464239	-1.638897	-0.060902
C	2.604811	-0.516302	0.021519
C	3.189842	0.785703	0.026208
C	4.597180	0.900940	-0.051956
C	1.189636	-0.592797	0.101291
C	0.342148	0.468770	0.183946
C	0.975066	1.715833	0.182617
C	2.325436	1.899535	0.109453
F	5.185995	2.097949	-0.052295
F	6.711209	-0.094069	-0.201718
F	5.619586	-2.546275	-0.212138
F	2.977409	-2.880036	-0.070827
F	2.826953	3.142014	0.116906
F	0.208012	2.826368	0.259506
Mg	-1.782922	0.278632	0.267529
C	-4.632973	1.067619	-0.157595
C	-4.209371	-1.379188	0.301067
C	-5.528096	1.514397	1.019961
C	-4.973653	-1.648552	1.616346
N	-3.699265	-0.009865	0.177819
C	-2.989642	-2.309812	0.303560
H	-2.390303	-2.168021	-0.604984

H	-2.359873	-2.126279	1.186707
H	-3.283987	-3.361915	0.342027
C	-5.100380	-1.748478	-0.901917
C	-5.517455	0.677679	-1.358988
C	-3.787765	2.284808	-0.551195
H	-3.177913	2.620780	0.299541
H	-3.124489	2.038204	-1.389614
H	-4.410325	3.130425	-0.855060
C	-6.169781	-0.691112	-1.172532
H	-6.740653	-0.958184	-2.066733
H	-6.887885	-0.658535	-0.346297
H	-6.277541	1.449433	-1.524487
H	-4.883405	0.645015	-2.254072
H	-5.559691	-2.729209	-0.734981
H	-4.459524	-1.833672	-1.788597
H	-6.297941	0.783290	1.266203
H	-4.916034	1.676096	1.912134
H	-6.036324	2.453609	0.777574
H	-5.136930	-2.722868	1.751622
H	-4.391597	-1.280225	2.466288
H	-5.950201	-1.165577	1.642508
F	0.655740	-1.839799	0.090649

3a···F7MgTMP

C	5.152251	0.551370	-1.217090
C	4.699839	-0.652256	-1.785601
C	3.375353	-0.972052	-1.754717
C	2.424878	-0.111221	-1.155067
C	2.888201	1.110592	-0.579602
C	4.269567	1.409478	-0.633649
C	1.040364	-0.397687	-1.034932
C	0.117040	0.377781	-0.408347
C	0.631223	1.564298	0.121629
C	1.940851	1.944379	0.052797
F	4.745672	2.537069	-0.102229
F	6.452029	0.830652	-1.259670

F	5.589217	-1.468578	-2.347047
F	3.004905	-2.131937	-2.302578
F	2.328117	3.099511	0.614162
F	-0.208620	2.395481	0.780272
Mg	-1.913987	-0.260845	-0.110436
C	-4.600598	0.743418	0.679196
C	-4.133867	0.823284	-1.791122
C	-5.864746	-0.141299	0.796400
C	-5.254008	-0.046740	-2.407347
N	-3.727277	0.406859	-0.447511
C	-2.908794	0.663039	-2.698343
H	-2.085240	1.298394	-2.354555
H	-2.567416	-0.382724	-2.704541
H	-3.134050	0.934752	-3.733302
C	-4.560998	2.305491	-1.816623
C	-5.018430	2.227471	0.641523
C	-3.789682	0.502626	1.959533
H	-3.535545	-0.561163	2.058051
H	-2.866892	1.097314	1.948457
H	-4.351012	0.786405	2.854157
C	-5.576549	2.629784	-0.722436
H	-5.808793	3.698965	-0.731975
H	-6.519956	2.107039	-0.914196
H	-5.749104	2.429313	1.433394
H	-4.129883	2.836930	0.850836
H	-4.960862	2.562639	-2.804227
H	-3.665779	2.919169	-1.654752
H	-6.610402	0.083848	0.034102
H	-5.592641	-1.197054	0.703126
H	-6.343486	0.002918	1.771007
H	-5.375628	0.180785	-3.471817
H	-4.996409	-1.106470	-2.313541
H	-6.221391	0.107914	-1.929816
F	0.623634	-1.579523	-1.567009
C	-3.078481	-3.022730	0.061738
H	-3.588867	-3.498804	0.903948

H	-3.776536	-2.338193	-0.421860
C	-1.375287	-2.763162	1.747130
H	-2.094259	-2.759880	2.572174
H	-1.103582	-3.794041	1.511920
O	-2.023438	-2.185175	0.593929
C	-0.156845	-1.956185	2.082878
C	1.094066	-2.336069	1.600509
C	-0.274739	-0.785752	2.834428
C	2.216865	-1.554045	1.847204
H	1.193624	-3.245653	1.017306
C	0.835310	0.012978	3.084393
H	-1.242559	-0.492191	3.230194
C	2.067399	-0.382699	2.578662
H	3.191480	-1.844373	1.472480
H	0.746154	0.927308	3.658210
C	-2.526216	-4.034851	-0.918457
H	-1.808943	-4.709700	-0.446971
H	-3.347174	-4.636540	-1.315282
H	-2.035939	-3.528575	-1.753043
Cl	3.471117	0.616806	2.876803